

NON-NEGATIVE LEAST SQUARES FOR HIGH-DIMENSIONAL LINEAR MODELS: CONSISTENCY AND SPARSE RECOVERY WITHOUT REGULARIZATION

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Least squares fitting is in general not useful for high-dimensional linear models, in which the number of predictors is of the same or even larger order of magnitude than the number of samples. Theory developed in recent years has coined a paradigm according to which sparsity-promoting regularization is regarded as a necessity in such setting. Deviating from this paradigm, we show that non-negativity constraints on the regression coefficients may be similarly effective as explicit regularization. For a broad range of designs with Gram matrix having non-negative entries, we establish bounds on the ℓ_2 -prediction error of non-negative least squares (NNLS) whose form qualitatively matches corresponding results for ℓ_1 -regularization. Under slightly stronger conditions, it is established that NNLS followed by hard thresholding performs excellently in terms of support recovery of an (approximately) sparse target, in some cases improving over ℓ_1 -regularization. A substantial advantage of NNLS over regularization-based approaches is the absence of tuning parameters, which is convenient from a computational as well as from a practitioner's point of view. Deconvolution of positive spike trains is presented as application.

1. Introduction. Consider the linear regression model

$$(1.1) \quad y = X\beta^* + \varepsilon,$$

where y is a vector of observations, $X \in \mathbb{R}^{n \times p}$ a design matrix, ε a vector of noise and β^* a vector of coefficients to be estimated. Throughout this paper, we are concerned with a high-dimensional setting in which the number of unknowns p is at least of the same order of magnitude as the number of observations n , i.e. $p = O(n)$ or even $p \gg n$, in which case one cannot hope to recover the target β^* if it does not satisfy one of various kinds of sparsity constraints, the simplest being that β^* is supported on $S = \{j : \beta_j^* \neq 0\}$, $|S| = s < n$. In this paper, we additionally assume that β^* is non-negative, i.e. $\beta^* \in \mathbb{R}_+^p$. This constraint is particularly relevant when modelling non-negative data, which emerge e.g. in the form of pixel intensity values of an image, time measurements, histograms or count data, economical quantities such as prices, incomes and growth rates. Non-negativity constraints occur naturally in numerous deconvolution and unmixing problems in diverse fields such as acoustics [29], astronomical imaging [2], hyperspectral imaging [1], genomics [28], proteomics

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[39], spectroscopy [20] and network tomography [31]; see [12] for a survey. As reported in these references, non-negative least squares (NNLS) yields at least reasonably good, sometimes even excellent results in practice, which may seem surprising in view of the simplicity of that approach. The NNLS problem is given by the quadratic program

$$(1.2) \quad \min_{\beta \succeq 0} \frac{1}{n} \|y - X\beta\|_2^2,$$

which is a convex optimization problem that can be solved efficiently [27]. Solid theoretical support for the empirical success of NNLS from a statistical perspective scarcely appears in the literature. An early reference is [20] dating back already two decades. The authors show that, depending on X and the sparsity of β^* , NNLS may have a 'super-resolution'-property that permits reliable estimation of β^* . Rather recently, sparse recovery of non-negative signals in a noiseless setting ($\varepsilon = 0$) has been studied in [5, 19, 48, 49]. One important finding of this body of work is that non-negativity constraints alone may suffice for sparse recovery, without the need to employ sparsity-promoting ℓ_1 -regularization as usually. The main contribution of the present paper is a transfer of this intriguing result to a more realistic noisy setup, contradicting the well-established paradigm that regularized estimation is necessary to cope with high dimensionality and to prevent over-adaptation to noise, thereby improving the understanding of the empirical success of NNLS. More specifically, we demonstrate that under suitable conditions on X , which are fulfilled, for example, if X has exclusively non-negative entries (a condition which is often met naturally for the applications listed above), hard thresholding of a minimizer $\hat{\beta}$ of (1.2) is an effective device for support recovery that may even improve over ℓ_1 -regularized least squares (lasso, [41]). Due to its combination of favourable computational and statistical properties, the lasso enjoys most popularity among various sparsity-promoting regularization schemes that have been proposed in recent years. As surveyed in [45], a series of strong theoretical guarantees concerning prediction, estimation of β^* and feature selection with the lasso have been established under various conditions on the design, some of which apply rather broadly. On the other hand, NNLS, as a pure fitting approach, avoids shortcomings of ℓ_1 -regularization. The bias caused by the regularization term negatively affects estimation of β^* with respect to the ℓ_∞ -norm and the performance for feature selection [52, 53, 56]. While different remedies have been proposed, such as subsequent thresholding for improved selection [33, 54], or the adaptive lasso [56], which addresses the bias, all these schemes, like *any* regularization-based scheme, entail careful tuning of at least one parameter. On the contrary, this is not required for NNLS and constitutes a definite advantage, particularly from a practical point of view. Parameter tuning by cross-validation increases the computational burden and may be error-prone if done by a grid search, since the grid could have an unfavourable range or a too small number of grid points. Apart from that, the use of cross-validation may not always be adequate in a fixed design setup, e.g. for the application in [39].

Outline and contributions of the paper. The paper significantly extends a previous conference publication [40]. Meinshausen has independently studied the performance of NNLS in a high-dimensional setting. His paper [31] contains an oracle property with respect to prediction and an ℓ_1 -bound for estimating

the coefficient vector. That work is related to ours in Section 2.5. Prediction performance is studied in Section 2, while the focus of our paper is on sparse recovery (Section 3). In particular, we study sparse recovery in an ℓ_∞ -sense and support recovery by thresholding. It is shown that the threshold can be chosen in an entirely data-driven way requiring only a single fit to the data as opposed to cross-validation.

We develop a common geometric framework hinging on large-margin separating hyperplanes within which the conditions required for our main results can be interpreted.

In Section 4, theory is complemented by illustrations and numerical results. It is outlined that NNLS can be useful for spike train deconvolution. Second, the performance with regard to sparse recovery compared to standard methods such as the lasso is investigated.

Proofs of statements not proven in the main manuscript are contained in the appendix.

Notation. We denote the usual ℓ_q -norm by $\|\cdot\|_q$. The cardinality of a set is denoted by $|\cdot|$. Let $J, K \subseteq \{1, \dots, m\}$ be index sets. For a matrix $A \in \mathbb{R}^{n \times m}$, A_J denotes the matrix one obtains by extracting the columns corresponding to J . For $j = 1, \dots, m$, A_j denotes the j -th column of A , while A^j denotes the j -th row. The matrix A_{JK} is the sub-matrix of A by extracting rows in J and columns in K . Likewise, for $v \in \mathbb{R}^m$, v_J is the sub-vector corresponding to J . The identity matrix is denoted by I and vectors of ones by $\mathbf{1}$. The symbols \preceq, \succeq and \prec, \succ denote componentwise inequalities and componentwise strict inequalities, respectively. In addition, for some matrix A , $A \succeq a$ means that all entries of A are at least equal to a scalar a . The non-negative orthant $\{x \in \mathbb{R}^m : x \succeq 0\}$ is denoted by \mathbb{R}_+^m . The standard simplex in \mathbb{R}^m , that is the set $\{x \in \mathbb{R}_+^m : \sum_{j=1}^m x_j = 1\}$ is denoted by T^{m-1} . Lower and uppercase c 's like $c, c', c_1, \bar{c}, \tilde{c}$ and $C, C', C_1, \bar{C}, \tilde{C}$ etc. denote positive constants not depending on the sample size n whose values may differ from line to line. In general, the positive integers $p = p_n$ and $s = s_n$ depend on n . Landau's symbols are denoted by $o(\cdot), O(\cdot), \Omega(\cdot)$. Asymptotics is to be understood w.r.t. a triangular array of observations $\{(X_n, y_n), X_n \in \mathbb{R}^{n \times p_n}\}$, $n = 1, 2, \dots$.

Normalization. If not stated otherwise, the design matrix X is considered as deterministic, having its columns normalized such that $\|X_j\|_2^2 = n$, $j = 1, \dots, p$.

General linear position. We say that the columns of X are in general linear position in \mathbb{R}^n if the following condition (GLP) holds

$$(1.3) \quad (\text{GLP}) : \quad \forall J \subset \{1, \dots, p\}, |J| \leq n : \quad X_J \lambda = 0 \implies \lambda = 0.$$

2. Prediction error. In the following section, NNLS is studied from the point of view of prediction. We first present several negative examples, where NNLS breaks down or overfits similarly as its unconstrained counterpart. We then derive a sufficient condition on X which allows us to show consistency of NNLS in a high-dimensional setting. Linking that condition to the given examples, we identify a transition regarding resistance to overfitting within the set of design matrices.

2.1. Minimum requirement on the design. In general, the non-negativity constraints in (1.2) may not be meaningful at all, given the fact that any least squares problem can be reformulated as a non-negative least squares problem

with an augmented design matrix $[X \ -X]$. More generally, NNLS can be as ill-posed as least squares if the following condition (\mathcal{H}) does not hold.

$$(2.1) \quad (\mathcal{H}) : \exists w \in \mathbb{R}^n \text{ such that } X^\top w \succ 0.$$

Condition (\mathcal{H}) requires the columns of X be contained in the interior of a half-space containing the origin. If (\mathcal{H}) fails to hold, $0 \in \text{conv}\{X_j\}_{j=1}^p$, so that there are infinitely many minimizers $\hat{\beta}$ of the NNLS problem (1.2). If additionally $p > n$ and the columns of X are in general linear position (condition (GLP) in (1.3)), 0 must be in the interior of $\text{conv}\{X_j\}_{j=1}^p$. It then follows that $\mathcal{C} = \mathbb{R}^n$, where $\mathcal{C} = \text{cone}\{X_j\}_{j=1}^p$ denotes the polyhedral cone generated by the columns of X . Consequently, the non-negativity constraints become vacuous and NNLS yields perfect fit for any observation vector y . In light of this, (\mathcal{H}) constitutes a necessary condition for a possible improvement of NNLS over ordinary least squares.

The half-space constraint (\mathcal{H}) is fulfilled, for example, if a subset of the rows of X takes only positive or only negative values, or if all columns of X are positively correlated, i.e. if all inner products of pairs of columns are non-negative.

On the contrary, random matrices having entries drawn i.i.d. from a zero-mean sub-Gaussian distribution, as they are typically considered in the compressed sensing literature [10, 11, 13] fail to satisfy (\mathcal{H}) with high probability if $p/n > 2$, which follows from Wendel's Theorem as pointed out in [19].

THEOREM 1. (Wendel, [37, 50])

Let X_1, \dots, X_p be i.i.d. random points in \mathbb{R}^n whose distribution is symmetric with respect to 0 and which assigns measure zero to every hyperplane through 0. Then for $X = [X_1 \ \dots \ X_p]$, it holds that

$$(2.2) \quad \mathbf{P}\left(X \text{ obeys } (\mathcal{H})\right) = \mathbf{P}(0 \leq B \leq n-1),$$

where B follows a binomial distribution with $p-1$ trials and probability of success equal to $\frac{1}{2}$.

For X as in above theorem, upper bounding (2.2) by means of Hoeffding's inequality implies that for $p/n > 2$,

$$(2.3) \quad \mathbf{P}\left(X \text{ obeys } (\mathcal{H})\right) \leq \exp\left(-n(p/n - 2)^2/2\right).$$

2.2. Overfitting under condition (\mathcal{H}) . Since NNLS is a pure fitting approach, over-adaptation to noise is a natural concern. Resistance to overfitting can be quantified in terms of $\frac{1}{n}\|X\hat{\beta}\|_2^2$ when y is a vector of Gaussian noise. The following two examples show that in general, condition (\mathcal{H}) is not sufficient to ensure that $\frac{1}{n}\|X\hat{\beta}\|_2^2 = o(1)$ with high probability. In Theorem 2 below, we consider random design whose realizations can be interpreted as generic representatives of the class of design matrices fulfilling condition (\mathcal{H}) .

THEOREM 2. Let $y = \varepsilon$, where ε has i.i.d. standard Gaussian entries, and let $X = \begin{pmatrix} v^\top \\ U \end{pmatrix}$ be independent of y , where v is an n -dimensional random

vector with i.i.d. entries from a zero-truncated standard Gaussian distribution and U is a random matrix of dimension $(n-1) \times p$ independent of v having i.i.d. standard Gaussian entries. Then, there exists a constant C_0 so that if $p/n \geq C_0 > 2$, it holds that $\frac{1}{n}\|X\hat{\beta}\|_2^2 = \Omega(1)$ with probability at least $1 - C \exp(-cn)$, $C, c > 0$.

Overfitting with orthonormal design. Suppose that X is orthonormal, i.e. $X^\top X = nI_p$. It is easy to see that NNLS also overfits in this case. Let $y = \varepsilon$ be a standard Gaussian random vector as above. The optimal coefficients can be given in closed form. We have that

$$\hat{\beta}_j = \max\{X_j^\top \varepsilon, 0\} / \|X_j\|_2^2, \quad j = 1, \dots, p,$$

so that the distribution of each component of $\hat{\beta}$ is given by a mixture of a point mass 0.5 at zero and a half-normal distribution. We conclude that $\frac{1}{n}\|X\hat{\beta}\|_2^2 = \frac{1}{n}\|\hat{\beta}\|_2^2$ is of the order $\Omega(p/n)$ with high probability. The fact that X is orthonormal is much stronger than the obviously necessary half-space constraint (\mathcal{H}) . In fact, as rendered more precisely below, orthonormal design turns out to be at the edge of the set of designs still leading to overfitting.

2.3. Designs with a 'self-regularizing' property. We now derive a sufficient condition X has to satisfy so that overfitting is prevented. That condition is referred to as *self-regularizing property*, expressing the fact that the design itself automatically generates a regularizing term. Denote by $\Sigma = \frac{1}{n}X^\top X$ the (scaled) Gram matrix of the columns of X . The NNLS problem for $y = \varepsilon$ can then be written as

$$(2.4) \quad \min_{\beta \succeq 0} -\frac{2}{n}\varepsilon^\top X\beta + \beta^\top \Sigma \beta.$$

Over-fitting can only be prevented by the quadratic term. Assuming that X satisfies (\mathcal{H}) , there exists a unit vector w and $h \succ 0$ such that $X^\top w = h$. Denote by $\Pi_w = ww^\top$ the orthogonal projection on w . We then have for all $\beta \succeq 0$

$$\begin{aligned} \beta^\top \Sigma \beta &= \frac{\beta^\top X^\top X \beta}{n} = \frac{\beta^\top X^\top \Pi_w X \beta}{n} + \frac{\beta^\top X^\top (I - \Pi_w) X \beta}{n} \\ &\geq \frac{\beta^\top X^\top w w^\top X \beta}{n} \geq \frac{(h^\top \beta)^2}{n} \geq \frac{h_{\min}}{n} (\mathbf{1}^\top \beta)^2, \end{aligned}$$

where h_{\min} is the minimum entry of h , i.e. the quadratic term in β can be lower bounded by its squared ℓ_1 -norm multiplied by some factor. The following condition results by optimizing that factor.

CONDITION 1. A design X with Gram matrix $\Sigma = \frac{1}{n}X^\top X$ is said to have a *self-regularizing property* if there exists a universal constant $\tau_0 > 0$ such that

$$(2.5) \quad \beta^\top \Sigma \beta \geq \tau_0^2 (\mathbf{1}^\top \beta)^2 \quad \forall \beta \succeq 0.$$

For given X , τ_0^2 can be obtained numerically as the optimal value of the quadratic program

$$(2.6) \quad \min_{\lambda \in T^{p-1}} \frac{1}{n} \|X\lambda\|_2^2, \quad T^{p-1} = \{\lambda \in \mathbb{R}_+^p : \mathbf{1}^\top \lambda = 1\},$$

which equals the squared Euclidean distance of the convex hull of the columns of X , scaled by $\frac{1}{\sqrt{n}}$, to the origin. Alternatively, τ_0 can be interpreted as *margin* of a maximum-margin *separating hyperplane* with normal vector w , which is determined from the optimization problem dual to (2.6):

$$(2.7) \quad \tau_0 = \max_{\tau, w} \tau \quad \text{subject to} \quad \frac{1}{\sqrt{n}} X^\top w \succeq \tau \mathbf{1}, \quad \text{and} \quad \|w\|_2 \leq 1.$$

The geometry as well as the duality of (2.6) and (2.7) parallels the construction principle of separating hyperplanes in the context of support vector machines, cf. e.g. [38], Sec. 7.2.

Condition (2.5) does not only rule out overfitting. It additionally gives rise to the following general bound on the ℓ_2 -prediction error of NNLS, where the assumption that the linear model is specified correctly, is not made. Instead, we only assume that there is a fixed target $f = (f_1, \dots, f_n)^\top$ to be approximated by a non-negative combination of the columns of X .

THEOREM 3. *Let $y = f + \varepsilon$, where $f \in \mathbb{R}^n$ is fixed and ε has i.i.d. zero-mean sub-Gaussian entries with parameter σ . Define*

$$\mathcal{E}^* = \min_{\beta \succeq 0} \frac{1}{n} \|X\beta - f\|_2^2, \quad \widehat{\mathcal{E}} = \frac{1}{n} \|X\widehat{\beta} - f\|_2^2.$$

Suppose that X satisfies Condition 1. Then, with probability no less than $1 - 2/p$, it holds that

$$(2.8) \quad \widehat{\mathcal{E}} \leq \mathcal{E}^* + \left(\frac{12\|\beta^*\|_1 + 16\sqrt{\mathcal{E}^*}}{\tau_0^2} \right) \sigma \sqrt{\frac{2 \log p}{n}} + \frac{64\sigma^2 \log p}{\tau_0^2 n},$$

for all $\beta^ \in \arg\min \frac{1}{n} \|X\beta - f\|_2^2$.*

2.4. Discussion.

Discussion of Condition 1. One might ask whether instead of Condition 1, which provides a lower bound on the quadratic form $\beta^\top \Sigma \beta$ for all non-negative vectors in terms of their ℓ_1 -norm, one could employ the following alternative: *There exists a universal constant $\eta > 0$ so that*

$$\beta^\top \Sigma \beta \geq \eta \|\beta\|_2^2 \quad \forall \beta \succeq 0.$$

However, this condition is in general too weak, since it is satisfied for orthonormal design with $\eta = 1$, for which NNLS overfits. On the other hand, orthonormal design does *not* obey Condition 1, because it leads to $\tau_0^2 = 1/n$ in (2.5). Likewise, the random design of Theorem 2 does not obey Condition 1 with high probability. In fact, with the same notation as in the theorem, one has

$$\beta^\top \Sigma \beta = \frac{\beta^\top U^\top U \beta}{n} + \frac{\beta^\top v v^\top \beta}{n}.$$

By Wendel's Theorem 1, for $p \geq 2.5n$, zero is contained in the convex hull of the columns of U with probability close to 1, so that τ_0^2 cannot be larger than $\|v\|_\infty^2/n$, which scales as $O(\log(p)/n)$ with high probability. These observations suggest that the scaling of τ_0^2 in (2.5) is a reasonable indicator for potential resistance to overfitting.

Examples of designs satisfying Condition 1.

Entry-wise positive lower bound on the Gram matrix. If $\Sigma \succeq \sigma_0 > 0$, then (2.5) holds with $\tau_0^2 = \sigma_0$. In particular, this is fulfilled if the columns of X are all strictly contained in the interior of an orthant of \mathbb{R}^n . This example suggests that orthonormal design marks the transition between overfitting and resistance to overfitting, respectively.

Band- or block structure with a positive lower bound. If $\Sigma \succeq 0$ and if the set of predictors indexed by $\{1, \dots, p\}$ can be partitioned into blocks B_1, \dots, B_K such that $\min_{1 \leq l \leq K} \frac{1}{n} X_{B_l}^\top X_{B_l} \succeq \sigma_0$, then

$$\min_{\beta \succeq 0} \beta^\top \Sigma \beta \geq \sum_{l=1}^K \beta_{B_l}^\top \frac{1}{n} X_{B_l}^\top X_{B_l} \beta_{B_l} \geq \sigma_0 \sum_{l=1}^K (\mathbf{1}^\top \beta_{B_l})^2 \geq \frac{\sigma_0}{K} (\mathbf{1}^\top \beta)^2.$$

In particular, as sketched in Figure 1, this applies to design matrices whose entries contain the function evaluations at points $\{u_i\}_{i=1}^n \subset [a, b]$ of non-negative functions such as splines, Gaussian kernels and related 'localized' functions traditionally used for data smoothing. If the points $\{u_i\}_{i=1}^n$ are placed evenly in $[a, b]$ then the corresponding Gram matrix effectively has a band structure. For instance, suppose that $u_i = i/n$, $i = 1, \dots, n$, and consider indicator functions of sub-intervals $\phi_j(u) = I\{u \in [(\mu_j - h) \vee a, (\mu_j + h) \wedge b]\}$, where $\mu_j \in [0, 1]$, $j = 1, \dots, p$, and $h = 1/K$ for some positive integer K . Setting $X = (\phi_j(u_i))_{1 \leq i \leq n, 1 \leq j \leq p}$ and partitioning the $\{\mu_j\}$ by dividing $[0, 1]$ into intervals $[0, h]$, $(h, 2h]$, \dots , $(1-h, 1]$ and accordingly $B_l = \{j : \mu_j \in ((l-1) \cdot h, l \cdot h]\}$, $l = 1, \dots, K$, we have that $\min_{1 \leq l \leq K} \frac{1}{n} X_{B_l}^\top X_{B_l} \succeq h$ such that property (2.5) holds with $\tau_0^2 = h/K = 1/K^2$.

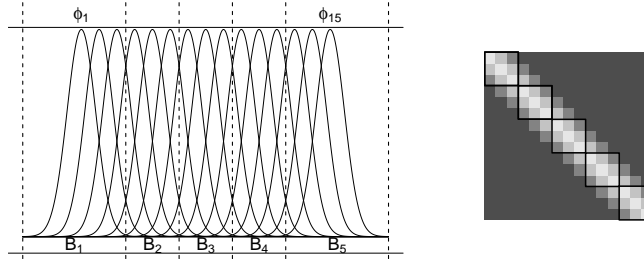


FIG 1. Block partitioning of 15 Gaussians into $K = 5$ blocks. The right part shows the corresponding pattern of the Gram matrix.

Discussion of Theorem 3. In Theorem 3, it is established that the ℓ_2 -prediction error of NNLS approaches that of the optimal non-negative combination of the columns of X provided $\|\beta^*\|_1 = o(\sqrt{n/\log p})$, which implies that NNLS can be consistent in a regime in which the number of predictors is nearly exponential in n . In that sense, NNLS constitutes a 'persistent procedure' in the spirit of Greenshtein and Ritov [25] who coined the notion of 'persistence' as distinguished from classical consistency with a fixed number of predictors. The authors study persistence of the lasso estimator $\hat{\beta}^{\ell_1}$, defined as a minimizer of

$$(2.9) \quad \min_{\beta} \frac{1}{n} \|y - X\beta\|_2^2 + \lambda \|\beta\|_1,$$

where $\lambda > 0$ is the regularization parameter. Interestingly, our Theorem 3 can be matched to a corresponding result for the lasso. If the linear model is correct, i.e. if $f = X\beta^*$ with $\beta^* \succeq 0$ and consequently $\mathcal{E}^* = 0$, the leading term of the bound (2.8) is of the order $O(\|\beta^*\|_1 \sqrt{\log(p)/n})$. The same rate – without any assumption on the design – is readily obtained for the lasso, using an argument that can essentially be found in [6]. Since $\hat{\beta}^{\ell_1}$ is a minimizer of (2.9), one has

$$\frac{1}{n} \|X(\hat{\beta}^{\ell_1} - \beta^*)\|_2^2 + \lambda \|\hat{\beta}^{\ell_1}\|_1 \leq \frac{2}{n} \varepsilon^\top X(\hat{\beta}^{\ell_1} - \beta^*) + \lambda \|\beta^*\|_1.$$

Choosing $\lambda = 2\lambda_0$, $\lambda_0 = \frac{2}{n} \|X^\top \varepsilon\|_\infty$, applying Hölder's inequality to the right hand side, using $\|\hat{\beta}^{\ell_1} - \beta^*\|_1 \leq \|\hat{\beta}^{\ell_1}\|_1 + \|\beta^*\|_1$ and re-arranging, it follows that $\frac{1}{n} \|X(\hat{\beta}^{\ell_1} - \beta^*)\|_2^2 \leq 3\lambda_0 \|\beta^*\|_1$. With ε as in Theorem 3, $\lambda_0 = O(\sqrt{\log(p)/n})$ with high probability, such that one ends up with a bound qualitatively equal to (2.8).

In [26], the problem of finding an optimal (in the sense of ℓ_2 -prediction error) convex combination out of a set of given regression functions is considered, which, in our setting would correspond to the additional constraint $\mathbf{1}^\top \beta = 1$. When setting $\|\beta^*\|_1 = 1$ in (2.8), the rate becomes qualitatively equal to the corresponding result in [26].

Remark. NNLS has been introduced as a tool for 'non-negative data'. In this context, the assumption of zero-mean noise in Theorem 3 is questionable. In case that the entries of ε have a positive mean, one can decompose ε into a constant term, which can be absorbed into the linear model, and a second term which has mean zero.

2.5. Near-optimal rate under the 'compatibility condition'. In this subsection, we relate our work to the recent paper by Meinshausen [31] who has independently studied the performance of NNLS for high-dimensional linear models. In [31], our Condition 1, which is termed 'positive eigenvalue condition' there, is combined with an assumption of an underlying sparse linear model and the 'compatibility condition' [44, 45], which yields a bound on $\|\hat{\beta} - \beta^*\|_1$ and an improved rate for the ℓ_2 -prediction error in the flavour of sparsity oracle inequalities previously derived for the lasso, see e.g. [3, 7, 9, 44]. These works show that the lasso may adapt to the underlying sparsity, since, under appropriate assumptions on the design, the ℓ_2 -prediction error may be only of the order $O(s \log(p)/n)$, where s is the number of non-zero entries of β^* . Apart from a logarithmic factor, that is what could be achieved if the support of β^* were known in advance. In the sequel, we state a result of that type.

CONDITION 2. [45] Let $S \subseteq \{1, \dots, p\}$, $|S| = s$ and $\alpha > 1$. Define

$$\mathcal{R}(\alpha, S) = \{\delta \in \mathbb{R}^p : \|\delta_{S^c}\|_1 \leq \alpha \|\delta_S\|_1\}.$$

We say that the design satisfies the (α, S) -compatibility condition if there exists a constant $\phi(\alpha, S)$ such that

$$(2.10) \quad \delta^\top \Sigma \delta \geq s^{-1} \phi(\alpha, S) \|\delta_S\|_1^2 \quad \forall \delta \in \mathcal{R}(\alpha, S).$$

The compatibility condition is slightly weaker than the corresponding restricted eigenvalue condition [3] which applies to random sub-Gaussian matrices for s sufficiently small in a broad sense [55].

THEOREM 4. Assume that $y = X\beta^* + \varepsilon$, where $\beta^* \succeq 0$ has support S , $|S| = s$, ε has i.i.d. sub-Gaussian entries with sub-Gaussian parameter σ . Further assume that X satisfies Condition 1 as well as the $(3/\tau_0^2, S)$ -compatibility condition. It then holds that

(2.11)

$$\|\widehat{\beta} - \beta^*\|_1 \leq \frac{64 s}{\tau_0^4 \phi\left(\frac{3}{\tau_0^2}, S\right)} \sqrt{\frac{2 \log(p)}{n}}, \quad \frac{1}{n} \|X\widehat{\beta} - X\beta^*\|_2^2 \leq \frac{128}{\tau_0^4 \phi\left(\frac{3}{\tau_0^2}, S\right)} \frac{s \log(p)}{n},$$

with probability no less than $1 - 2/p$.

A similar result with better constants is shown in [31]. However, in [31] a lower bound on the minimum non-zero coefficient of β^* is required, which is not natural and does not appear in corresponding results for the lasso. One can deduce sparse recovery by thresholding as an immediate corollary of Theorem 4, which provides an ℓ_1 -bound for the estimation of β^* . Considerably stronger results concerning sparse recovery are implied by the ℓ_∞ -bounds of the following second part of the paper.

3. Sparse recovery. Within this section, we focus on the situation where β^* is at least approximately sparse. We argue that NNLS may achieve a near-optimal rate for estimating β^* in sup-norm, which makes thresholding an effective device for support recovery.

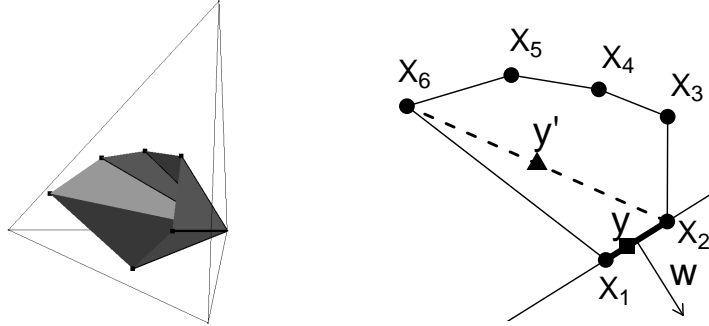


FIG 2. Left panel: Cone $\mathcal{C} = X\mathbb{R}_+^p \subset \mathbb{R}_+^3$ for $p = 6$. Right panel: A slice of \mathcal{C} . The columns of X are indicated by round dots. The face containing y is depicted by a bold black segment which is part of a solid line representing the separating hyperplane with corresponding normal vector w .

3.1. Geometry. For the rest of the paper, we assume that the columns of X are in general linear position, i.e. that condition (GLP) in (1.3) holds. We start by studying the noiseless ($\varepsilon = 0$) and exactly sparse case. Figure 2 provides some intuition for the problem on the basis of geometric ideas used and developed in [15, 16, 19, 48]. The left panel displays a polyhedral cone $\mathcal{C} = \text{cone}\{X_j\}_{j=1}^p$, $p = 6$ contained in \mathbb{R}_+^3 . In the given example, the vector y (represented by a square) is contained in the boundary of \mathcal{C} , whereas y' (represented by a triangle) is contained in the interior of \mathcal{C} . Consider now the two underdetermined linear systems of equations with non-negativity constraints

$$y = X\beta \quad \text{sb.t. } \beta \succeq 0, \quad y' = X\beta' \quad \text{sb.t. } \beta' \succeq 0.$$

It is clear from the picture that β is determined uniquely, whereas β' is not. The observation to be made here is that y is contained in a two-dimensional *face* of \mathcal{C} . In general, given $F \subseteq \{1, \dots, p\}$, $F \neq \emptyset$, $\mathcal{C}_F = \text{cone}\{X_j\}_{j \in F}$, which is the polyhedral cone generated by the sub-matrix X_F , is called a face of \mathcal{C} if there exists $w \in \mathbb{R}^n$ such that $\langle X_j, w \rangle = 0$, $j \in F$, and $\langle X_j, w \rangle > 0$, $j \notin F$. In other words, there exists a hyperplane containing the origin separating the cones \mathcal{C}_F and \mathcal{C}_{F^c} . Given this definition, we conclude with the following statement regarding support recovery in the noiseless and exactly sparse case.

PROPOSITION 1. *Let $y = X\beta^*$, where $\beta^* \succeq 0$ has support S , $|S| = s$. The constrained linear system $X\beta = y$ s.t. $\beta \succeq 0$, has β^* as its unique solution if \mathcal{C}_S is a face of \mathcal{C} . Conversely, if \mathcal{C}_S is not a face of \mathcal{C} , there exists $\beta^* \succeq 0$ supported only on S such that uniqueness fails to hold.*

PROOF. By definition, since \mathcal{C}_S is a face of \mathcal{C} , there is a hyperplane separating \mathcal{C}_S from \mathcal{C}_{S^c} , i.e. there exists $w \in \mathbb{R}^n$ such that $\langle X_j, w \rangle = 0$, $j \in S$, $\langle X_j, w \rangle > 0$, $j \in S^c$. Assume that there is a second solution $\beta^* + \delta$, $\delta \neq 0$. Expand $X_S(\beta_S^* + \delta_S) + X_{S^c}\delta_{S^c} = y$. Multiplying both sides by w^\top yields $\sum_{j \in S^c} \langle X_j, w \rangle \delta_j = 0$. Since $\beta_{S^c}^* = 0$, feasibility requires $\delta_j \geq 0$, $j \in S^c$. All inner products within the sum are positive, concluding that $\delta_{S^c} = 0$. General position of the columns of X (1.3) implies that $\delta_S = 0$.

If \mathcal{C}_S is not a face of \mathcal{C} , then the convex hulls generated by $\{X_j\}_{j \in S}$ and $\{X_j\}_{j \in S^c}$, respectively, have a non-empty intersection. \square

To achieve robustness in the presence of noise, we strengthen the notion of a face by quantifying the amount of separation. The following definition naturally extends (2.7).

DEFINITION 1. *Let $S \subset \{1, \dots, p\}$, $S \neq \emptyset$, be given. The separating hyperplane constant (with respect to S) is defined as optimal value of the quadratic program*

$$(3.1) \quad \begin{aligned} \tau(S) &= \max_{\tau, w} \tau \\ \text{subject to } & \frac{1}{\sqrt{n}} X_S^\top w = 0, \quad \frac{1}{\sqrt{n}} X_{S^c}^\top w \succeq \tau \mathbf{1}, \quad \|w\|_2 \leq 1. \end{aligned}$$

Clearly, $\tau(S) > 0$ if and only if \mathcal{C}_S is a face of \mathcal{C} . In view of

$$\min_{j \in S^c} \frac{1}{\sqrt{n}} X_j^\top w \geq \tau \iff \min_{\lambda \in T^{p-s-1}} \lambda^\top \frac{1}{\sqrt{n}} X_{S^c}^\top w \geq \tau,$$

where $T^{p-s-1} = \{\lambda \in \mathbb{R}_+^{p-s} : \lambda^\top \mathbf{1} = 1\}$ is the standard simplex in \mathbb{R}^{p-s} , it is easy to see that $\tau(S)$ can be defined equivalently in terms of the following optimization problem dual to (3.1).

$$(3.2) \quad \tau(S) = \min_{\theta \in \mathbb{R}^s, \lambda \in T^{p-s-1}} \frac{1}{\sqrt{n}} \|X_S \theta - X_{S^c} \lambda\|_2,$$

i.e. $\tau(S)$ equals the distance of the subspace spanned by the support columns to the convex hull of the off-support columns. In the following, we denote by Π_S and Π_S^\perp the orthogonal projections on the subspace spanned by $\{X_j\}_{j \in S}$

and its orthogonal complement, respectively, and set $Z = \Pi_S^\perp X_{S^c}$. We can then compactly rewrite (3.2) as

$$(3.3) \quad \tau^2(S) = \min_{\lambda \in T^{p-s-1}} \frac{1}{n} \|Z\lambda\|_2^2 = \min_{\lambda \in T^{p-s-1}} \lambda^\top \frac{1}{n} Z^\top Z \lambda.$$

From (3.3), we see that the separating hyperplane constant is nothing else than the constant τ_0 in Condition 1, applied with respect to the matrix Z and the linear space orthogonal to that spanned by the support columns. This observation will permit us to carry over parts of the reasoning underlying the results of the preceding section to establish robustness of sparse recovery.

3.2. A general robust sparse recovery result. Equipped with the separating hyperplane constant, we are in position to state the following result, which asserts robustness of sparse recovery with respect to additive noise and approximate sparsity. Writing $\beta_{(1)}^* \geq \dots \geq \beta_{(p)}^* \geq 0$ for the sequence of ordered coefficients, let $S = \{j : \beta_j^* \geq \beta_{(s)}^*\}$ be the set of the s largest coefficients of β^* (for simplicity, assume that there are no ties). For the results that follow, we think of $\|\beta_{S^c}^*\|_1$ being considerably smaller than the entries of β_S^* . The standard case of exact sparsity in which S equals the support of β^* is covered by setting $\|\beta_{S^c}^*\|_1 = 0$. In order to state the following Theorem 5, the following quantities are required.

$$(3.4) \quad \beta_{\min}(S) = \min_{j \in S} \beta_j^*, \quad K(S) = \max_{\|v\|_\infty=1} \|\Sigma_S^{-1} v\|_\infty, \quad \phi_{\min}(S) = \min_{\|v\|_2=1} \|\Sigma_S v\|_2.$$

THEOREM 5. *Given the linear model $y = X\beta^* + \varepsilon$, where $\beta^* \succeq 0$ and ε has i.i.d. zero-mean sub-Gaussian entries with sub-Gaussian parameter σ . Set*

$$b = \frac{2\|\beta_{S^c}^*\|_1 + 4\sigma\sqrt{\frac{2\log p}{n}}}{\tau^2(S)}, \quad \tilde{b} = (b + \|\beta_{S^c}^*\|_1) K(S) + \frac{2\sigma}{\sqrt{\phi_{\min}(S)}} \sqrt{\frac{2\log p}{n}}.$$

If $\beta_{\min}(S) > \tilde{b}$, then the NNLS estimator $\hat{\beta}$ has the following properties with probability no less than $1 - 4/p$:

$$\|\hat{\beta}_{S^c}\|_1 \leq b \quad \text{and} \quad \|\hat{\beta}_S - \beta_S^*\|_\infty \leq \tilde{b}.$$

Roughly speaking, Theorem 5 guarantees that if the columns corresponding to S are 'sufficiently separated' from those in S^c as quantified by $\tau^2(S)$, then $\|\hat{\beta}_{S^c}\|_1$ can be upper bounded in terms of $\|\beta_{S^c}^*\|_1$, the noise level and $\tau^2(S)$, provided that the entries of β_S^* are all large enough. Since, as discussed below, $\tau^2(S)$ cannot be expected to be larger than $\Omega(s^{-1})$ and $K(S) = \sqrt{s} \{\phi_{\min}(S)\}^{-1}$ (cf. (3.4)) in the worst case, the bound on $\|\hat{\beta}_S - \beta_S^*\|_\infty$ is sub-optimal because of its dependence on s . This will be improved in Section 3.6.

3.3. Analysis by decomposition. Theorem 5 follows from a decomposition of the NNLS problem into two sub-problems corresponding to S and S^c , respectively. The latter is tackled by using the separating hyperplane constant. That decomposition, which is detailed below, serves as our main proof technique that is used for several subsequent results as well.

Key lemmas. The first lemma is immediate from the KKT optimality conditions of the NNLS problem. Its proof is hence omitted.

LEMMA 1. $\hat{\beta}$ is a minimizer of (1.2) if and only if there exists $F \subseteq \{1, \dots, p\}$ such that

$$\frac{1}{n}X_j^\top(y - X\hat{\beta}) = 0, \text{ and } \hat{\beta}_j > 0, j \in F, \quad \frac{1}{n}X_j^\top(y - X\hat{\beta}) \leq 0, \text{ and } \hat{\beta}_j = 0, j \in F^c.$$

Lemma 1 implies that the NNLS estimator $\hat{\beta}$ can be obtained from the following restricted least squares problem, once an *active set* F is known:

$$\min_{\beta_F} \frac{1}{n} \|y - X\beta\|_2^2 \quad \text{subject to } \beta_{F^c} = 0.$$

Note that F can always be chosen so that $|F| \leq n$, and that F is determined uniquely whenever $y \notin \mathcal{C}$ (and the columns of X are in general linear position (1.3)), in which case $X\hat{\beta}$, the projection of y on \mathcal{C} , is contained in the boundary of \mathcal{C} , i.e. in a lower-dimensional face \mathcal{C}_F of \mathcal{C} .

The next lemma is crucial, since it permits us to decouple $\hat{\beta}_S$ from $\hat{\beta}_{S^c}$.

LEMMA 2. Consider the two non-negative least squares problems

$$(P1) : \min_{\beta^{(P1)} \succeq 0} \frac{1}{n} \|\xi + Z\beta_{S^c}^* - Z\beta^{(P1)}\|_2^2, \quad \xi = \Pi_S^\perp \varepsilon, \quad Z = \Pi_S^\perp X_{S^c}.$$

$$(P2) : \min_{\beta^{(P2)} \succeq 0} \frac{1}{n} \|\Pi_S \varepsilon + \Pi_S X_{S^c} \beta_{S^c}^* + X_S \beta_S^* - X_S \beta^{(P2)} - \Pi_S X_{S^c} \hat{\beta}^{(P1)}\|_2^2$$

with minimizers $\hat{\beta}^{(P1)}$ of (P1) and $\hat{\beta}^{(P2)}$ of (P2), respectively. If $\hat{\beta}^{(P2)} \succ 0$, then setting $\hat{\beta}_S = \hat{\beta}^{(P2)}$ and $\hat{\beta}_{S^c} = \hat{\beta}^{(P1)}$ yields a minimizer $\hat{\beta}$ of the non-negative least squares problem (1.2).

PROOF. The NNLS objective is split into two parts in the following way:

$$(3.5) \quad \frac{1}{n} \|y - X\beta\|_2^2 = \frac{1}{n} \|\Pi_S y - X_S \beta_S - \Pi_S X_{S^c} \beta_{S^c}\|_2^2 + \frac{1}{n} \|\xi + Z\beta_{S^c}^* - Z\beta_{S^c}\|_2^2,$$

Separate minimization of the second summand on the r.h.s. of (3.5) yields $\hat{\beta}^{(P1)}$. Substituting $\hat{\beta}^{(P1)}$ for β_{S^c} in the first summand, and minimizing the latter amounts to solving (P2). In view of Lemma 1, if $\hat{\beta}^{(P2)} \succ 0$, it coincides with the unconstrained least squares estimator (3.5) corresponding to problem (P2). This implies that the optimal value of (P2) must be zero, because the observation vector $\Pi_S y$ of the non-negative least squares problem (P2) is contained in the column space of X_S . Since the second summand in (3.5) corresponding to (P1) cannot be made smaller than by separate minimization, we have minimized the non-negative least squares objective. The result follows by expanding $\Pi_S y = \Pi_S \varepsilon + \Pi_S X_{S^c} \beta_{S^c}^* + X_S \beta_S^*$. \square

Proof of Theorem 5.

Consider problem (P1) of Lemma 1.

Step 1: Controlling $\|\hat{\beta}^{(P1)}\|_1$ via $\tau^2(S)$. Since $\hat{\beta}^{(P1)}$ is a minimizer and 0 is a feasible for (P1), we have

$$\frac{1}{n} \|\xi + Z\beta_{S^c}^* - Z\beta_{S^c}\|_2^2 \leq \frac{1}{n} \|\xi + Z\beta_{S^c}^*\|_2^2,$$

which implies that

$$(3.6) \quad \begin{aligned} (\widehat{\beta}^{(P1)})^\top \frac{1}{n} Z^\top Z \widehat{\beta}^{(P1)} &\leq \|\widehat{\beta}^{(P1)}\|_1 \left(A + 2 \left\| \frac{1}{n} Z^\top Z \beta_{S^c}^* \right\|_\infty \right), \quad A = \max_{1 \leq j \leq (p-s)} \frac{2}{n} |Z_j^\top \xi|. \\ &\leq \|\widehat{\beta}^{(P1)}\|_1 (A + 2\|\beta_{S^c}^*\|_1) \end{aligned}$$

As observed in (3.3), $\tau^2(S) = \min_{\lambda \in T^{p-s-1}} \lambda^\top \frac{1}{n} Z^\top Z \lambda$, s.t. the l.h.s. can be lower bounded via

$$(3.7) \quad (\widehat{\beta}^{(P1)})^\top \frac{1}{n} Z^\top Z \widehat{\beta}^{(P1)} \geq \tau^2(S) \|\widehat{\beta}^{(P1)}\|_1^2.$$

Combining (3.6) and (3.7), we have $\|\widehat{\beta}^{(P1)}\|_1 \leq (A + 2\|\beta_{S^c}^*\|_1)/\tau^2(S)$.

Step 2: Back-substitution into (P2). Equipped with the bound just derived, we insert $\widehat{\beta}^{(P1)}$ into problem (P2) of Lemma 2, and show that in conjunction with the assumptions made for the minimum support coefficient $\beta_{\min}(S)$, the *ordinary* least squares estimator corresponding to (P2)

$$\bar{\beta}^{(P2)} = \underset{\beta^{(P2)}}{\operatorname{argmin}} \frac{1}{n} \|\Pi_S y - X_S \beta^{(P2)} - \Pi_S X_{S^c} \widehat{\beta}^{(P1)}\|_2^2$$

has only positive components. Lemma 2 then yields $\bar{\beta}^{(P2)} = \widehat{\beta}^{(P2)} = \widehat{\beta}_S$. Using the closed form expression for the ordinary least squares estimator, one obtains

$$(3.8) \quad \begin{aligned} \bar{\beta}^{(P2)} &= \frac{1}{n} \Sigma_{SS}^{-1} X_S^\top \Pi_S y \\ &= \frac{1}{n} \Sigma_{SS}^{-1} X_S^\top (X_S \beta_S^* + \Pi_S \varepsilon - \Pi_S X_{S^c} (\widehat{\beta}^{(P1)} - \beta_{S^c}^*)) \\ &= \beta_S^* + \frac{1}{n} \Sigma_{SS}^{-1} X_S^\top \varepsilon - \Sigma_{SS}^{-1} \Sigma_{SS^c} (\widehat{\beta}^{(P1)} - \beta_{S^c}^*). \end{aligned}$$

It remains to control the two terms $A_S = \frac{1}{n} \Sigma_{SS}^{-1} X_S^\top \varepsilon$ and $\Sigma_{SS}^{-1} \Sigma_{SS^c} (\widehat{\beta}^{(P1)} - \beta_{S^c}^*)$. For the second term, we have

$$(3.9) \quad \begin{aligned} \|\Sigma_{SS}^{-1} \Sigma_{SS^c} (\widehat{\beta}^{(P1)} - \beta_{S^c}^*)\|_\infty &\leq \max_{\|v\|_\infty=1} \|\Sigma_{SS}^{-1} v\|_\infty \|\Sigma_{SS^c} (\widehat{\beta}^{(P1)} - \beta_{S^c}^*)\|_\infty \\ &\stackrel{(3.4)}{\leq} K(S) (\|\widehat{\beta}^{(P1)}\|_1 + \|\beta_{S^c}^*\|_1). \end{aligned}$$

Step 3: Putting together the pieces. The two random terms A and A_S are maxima of a finite collection of linear combinations of sub-Gaussian random variables so that (A.2) in Appendix A can be applied by estimating Euclidean norms. For A , we use that $\|Z_j\|_2 = \|\Pi_S^\perp X_j\|_2 \leq \|X_j\|_2$ for all j . Second, we have

$$(3.10) \quad A_S = \max_{1 \leq j \leq s} \frac{|v_j^\top \varepsilon|}{n}, \quad v_j = X_S \Sigma_{SS}^{-1} e_j, \quad j = 1, \dots, s,$$

where e_j denotes the j -th canonical basis vector. One has

$$\max_{1 \leq j \leq s} \|v_j\|_2^2 = \max_{1 \leq j \leq s} e_j^\top \Sigma_{SS}^{-1} X_S^\top X_S \Sigma_{SS}^{-1} e_j \stackrel{(3.4)}{\leq} \frac{n}{\phi_{\min}(S)}.$$

It follows that the event

$$\left\{ A \leq 4\sigma \sqrt{\frac{2 \log p}{n}} \right\} \cap \left\{ A_S \leq \frac{2\sigma}{\sqrt{\phi_{\min}(S)}} \sqrt{\frac{2 \log p}{n}} \right\}$$

holds with probability no less than $1 - 4/p$. Conditional on that event, it follows that

$$\|\beta^* - \bar{\beta}^{(P2)}\|_\infty \leq (b + \|\beta_{S^c}^*\|_1)K(S) + \frac{2\sigma}{\sqrt{\phi_{\min}(S)}}\sqrt{\frac{2\log p}{n}},$$

with b as in Theorem 5, and hence, using the lower bound on $\beta_{\min}(S)$, that $\bar{\beta}^{(P2)} = \hat{\beta}_S \succ 0$ and thus also that $\hat{\beta}^{(P1)} = \hat{\beta}_{S^c}$. \square

3.4. Uniqueness of solution. Uniqueness of the NNLS solution in the noisy case may follow in the form of corollaries to Theorems 3 and 5 when combined with the observation made after Lemma 1, namely that uniqueness is implied by $y \notin \mathcal{C}$.

COROLLARY 1. *Consider the setting of Theorem 3 with $\mathcal{E}^* = 0$. If $\frac{1}{n}\|X\hat{\beta} - X\beta^*\|_2^2 \rightarrow 0$ in probability as $n \rightarrow \infty$, then $\hat{\beta}$ is unique with probability tending to one.*

PROOF. Suppose first that $y \notin \mathcal{C}$, then $X\hat{\beta}$, the projection of y on \mathcal{C} , is contained in its boundary, i.e. in a lower-dimensional face. Using general position of the columns of X (1.3), Proposition 1 implies that $\hat{\beta}$ is unique. If y were already contained in \mathcal{C} , one would have $y = X\hat{\beta}$ and hence

$$(3.11) \quad \frac{1}{n}\|X\beta^* - X\hat{\beta}\|_2^2 = \frac{1}{n}\|X\beta^* - y\|_2^2 = \frac{1}{n}\|\varepsilon\|_2^2 = \Omega(1), \text{ with high probability,}$$

using concentration of the norm of the sub-Gaussian random vector ε . However, (3.11) contradicts the assumption that $\frac{1}{n}\|X\beta^* - X\hat{\beta}\|_2^2 \rightarrow 0$ in probability. \square

Note that $\hat{\beta}$ may be unique even though in the absence of noise the underdetermined linear system $X\beta = X\beta^*$ subject to $\beta \succeq 0$ may have multiple solutions. By concentration of measure, the sub-Gaussian noise vector ε is contained in a set $S_\varepsilon = \{v \in \mathbb{R}^n : c\sqrt{n} \leq \|v\|_2 \leq C\sqrt{n}\}$ with high probability. If the intersection $(X\beta^* + S_\varepsilon) \cap \mathcal{C}$ has small volume, y may in fact be no longer contained in \mathcal{C} .

Alternatively, a condition for uniqueness can be inferred from the decomposition of the previous subsection.

COROLLARY 2. *In the setting of Theorem 5, if it holds that*

$$\frac{\|\beta_{S^c}^*\|_1}{\tau^2(S)}\sqrt{\frac{\log p}{n}} + \frac{\log p}{\tau^2(S)n} \rightarrow 0 \text{ as } n \rightarrow \infty,$$

and that $s < \frac{1}{2}n$, then $\hat{\beta}$ is unique with probability tending to one.

PROOF. Observe that $y \in \mathcal{C}$ implies that $\frac{1}{n}\|y - X\hat{\beta}\|_2^2 = 0$ and hence also that $\frac{1}{n}\|\xi + Z\beta_{S^c}^* - Z\hat{\beta}_{S^c}\|_2^2 = 0$ (cf. (3.5)), which in turn implies that $\frac{1}{n}\|\xi\|_2^2 = \frac{1}{n}\|Z(\beta_{S^c}^* - \hat{\beta}_{S^c})\|_2^2$. Moreover, $\frac{1}{n}\|y - X\hat{\beta}\|_2^2 = 0$ implies that $\hat{\beta}_{S^c}$ is a minimizer of the sub-problem (P1) of Lemma 2, and since $\beta_{S^c}^*$ is a feasible solution of (P1), it holds that that

$$\frac{1}{n}\|Z(\beta_{S^c}^* - \hat{\beta}_{S^c})\|_2^2 \leq \frac{2}{n}\xi^\top Z(\hat{\beta}_{S^c} - \beta_{S^c}^*) \leq \frac{2}{n}\|Z^\top \xi\|_\infty(\|\beta_{S^c}^*\|_1 + \|\hat{\beta}_{S^c}\|_1).$$

Inserting the bound on $\|\widehat{\beta}_{S^c}\|_1$ of Theorem 5 and using that $\frac{1}{n}\|Z^\top \xi\|_\infty = O(\sqrt{\log(p)/n})$ with high probability, the assumption of the corollary implies that $\frac{1}{n}\|Z(\beta_{S^c}^* - \widehat{\beta}_{S^c})\|_2^2$ tends to zero, which contradicts $\frac{1}{n}\|\xi\|_2^2 = \frac{1}{n}\|Z(\beta_{S^c}^* - \widehat{\beta}_{S^c})\|_2^2$, since $\frac{1}{n}\|\xi\|_2^2 = \frac{1}{n}\|\Pi_S^\perp \varepsilon\|_2^2 = \Omega(1)$ with high probability, using that $s < \frac{1}{2}n$. \square

By removing dependence on $\|\beta_S^*\|_1$, Corollary 2 may constitute a considerable improvement over Corollary 1. The latter follows from Theorem 3, where no further assumption about β^* or geometric aspects of \mathcal{C} like the separating hyperplane constant $\tau(S)$ are made. If $\tau^2(S) = \Omega(s^{-1})$ (the scaling of $\tau^2(S)$ will be discussed in the next subsection) and $\|\beta_{S^c}^*\|_1 = 0$, the condition of Corollary 2 becomes $s \log(p)/n \rightarrow 0$, which is typically regarded to be necessary to cope with high-dimensional linear models in the presence of noise, e.g. [47].

3.5. Scaling of $\tau^2(S)$. In this subsection, we investigate the scaling of $\tau^2(S)$, the quantity our analysis crucially depends on. It is shown that for what we term 'equi-correlation-like' designs, which comprises a broad class of random designs that will here serve as proxy for general non-negative designs, $\tau^2(S)$ scales favourably as $\Omega(s^{-1})$, minus a deviation term, which has moderate dependence on p .

Equi-correlation-like designs. Suppose that X is such that $\Sigma = (1 - \rho)I + \rho \mathbf{1}\mathbf{1}^\top$, $0 < \rho < 1$. It is then easy to compute (cf. Appendix E) that for any $S \subset \{1, \dots, p\}$

$$(3.12) \quad \tau^2(S) = \tau^2(s) = \frac{(1 - \rho)\rho}{(s - 1)\rho + 1} + \frac{1 - \rho}{p - s} = \Omega(s^{-1}).$$

The fact that Σ has exactly the form given above, requires that $n = p$, i.e. it is not a suitable model for the high-dimensional case where $n < p$. Therefore, we instead look more closely at the following class of *random* designs (previously, X has always been considered fixed) whose population Gram matrix $\Sigma^* = \mathbf{E}[\frac{1}{n}X^\top X]$ has equi-correlation structure after proper re-scaling of the columns of X . More specifically, we consider the following ensemble of random matrices (3.13)

$$\text{Ens}_+ : X = (x_{ij})_{\substack{1 \leq i \leq n, \\ 1 \leq j \leq p}}, \{x_{ij}\} \text{ i.i.d. from a sub-Gaussian distribution on } \mathbb{R}_+.$$

Among others, the class of sub-Gaussian distributions on \mathbb{R}_+ encompasses all distributions on a bounded set on \mathbb{R}_+ , e.g. the family of beta distributions (with the uniform distribution as special case) on $[0, 1]$, Bernoulli distributions on $\{0, 1\}$ or more generally distributions on positive integers $\{0, 1, \dots, K\}$. For all random matrices belonging to the class (3.13), the corresponding population Gram matrix Σ^* can be put into equi-correlation structure by re-scaling. Denoting the mean of the entries and their squares by μ and μ_2 , respectively, we have $\Sigma^* = (\mu_2 - \mu^2)I + \mu^2 \mathbf{1}\mathbf{1}^\top$ such that re-scaling by $1/\sqrt{\mu_2}$ leads to equi-correlation with $\rho = \mu^2/\mu_2$.

$\tau^2(S)$ for equi-correlation-like designs. To obtain a lower bound on $\tau^2(S)$ for random designs from Ens_+ , one additionally has to take into account the deviation between Σ and Σ^* . Using tools from non-asymptotic random matrix theory, we show that the deviation is moderate, of the order $O(\sqrt{\log(p)/n})$.

THEOREM 6. Consider the random matrix ensemble Ens_+ . Let the rows of the random matrix X be scaled in a fashion that $\mathbf{E} \left[\frac{1}{n} X^\top X \right] = (1 - \rho)I + \rho \mathbf{1}\mathbf{1}^\top$ for some $\rho \in (0, 1)$. Fix an $S \subset \{1, \dots, p\}$, $|S| \leq s$. Then there exists constants $c, c_1, c_2, c_3, C, C' > 0$ such that for all $n \geq C \log(p)s^2$,

$$(3.14) \quad \tau^2(S) \geq c \frac{1}{s} - C' \sqrt{\frac{\log p}{n}}$$

with probability no less than $1 - 3/p - \exp(-c_1 n) - 2 \exp(-c_2 \log p) - \exp(-c_3 \log^{1/2}(p)s)$.

Theorem 6 asserts that the deviation of $\tau^2(S)$ from its population counterpart is well-controlled provided n, p, s are related by $n > C \log(p)s^2$. While this is encouraging, because it indicates that $\tau^2(S)$ is stable under random perturbations of the Gram matrix, the result is still too pessimistic, as can be seen from numerical experiments whose results are reported below. In the numerical study conducted, $n = 500$ is fixed and $p \in (1.2, 1.5, 2, 3, 5, 10) \cdot n$ and $s \in (0.01, 0.025, 0.05, 0.1, 0.15, 0.2, 0.25, 0.3, 0.4, 0.5) \cdot n$ vary. For each combination of (p, s) , as representative of Ens_+ , a random matrix of dimension $n \times p$ whose entries follow a uniform distribution on $[0, 1]$, is drawn and re-scaled such that the population Gram matrix has equi-correlation structure with parameter $\rho = 3/4$. We set $S = \{1, \dots, s\}$ and compute $Z = (I - \Pi_S)X_{S^c}$ using a QR decomposition of X_S and then solve the quadratic program $\min_{\lambda \in T^{p-s-1}} \lambda^\top \frac{1}{n} Z^\top Z \lambda$ with value $\tau^2(S)$ by means of an interior point method [4]. For each combination of (p, s) , 100 replications are performed. Figure 3 displays the averages obtained for $\tau^2(S)$ over these 100 replications. It is revealed that n does not have to be significantly larger than s as suggested by Theorem 6. In fact, even for s/n as large as 0.3, $\tau^2(S)$ is sufficiently bounded away from zero as long as p is not dramatically larger than n ($p/n = 10$). For $s/n > 0.3$ while simultaneously $p/n > 5$, $\tau^2(S)$ is numerically zero. Indeed, Figure 3 shows that there is a distinct region in the $(n/p, s/n)$ -plane where one cannot hope for sparse recovery. This is in accordance with the phase transition characterized by Donoho and Tanner [15–17, 19] regarding the proportion of faces of polytopes that continue to be faces after a random projection into a lower-dimensional space. While we have only considered a specific instance of the class Ens_+ , it is unlikely – not least because of the findings in [18] – that the results should depend on the specific probability distribution of the entries, provided the parameter ρ remains unchanged.

3.6. *Convergence in sup-norm and support recovery by thresholding.* In this section, we argue that under appropriate conditions, the NNLS estimator may achieve a near-optimal rate of convergence in sup-norm, i.e. it may hold that $\|\hat{\beta} - \beta^*\|_\infty = O(\sqrt{\log(p)/n})$ with high probability, in which case the set S of large coefficients can be effectively recovered by hard thresholding.

Sup-norm error of least squares and the smallest singular values of square matrices. Suppose that $n = p$ and that the columns of X are linearly independent. Given observations $y = X\beta^* + \varepsilon$ as in Theorem 5, a bound on $\|\bar{\beta} - \beta^*\|_\infty$, where $\bar{\beta}$ denotes the *ordinary* least squares estimator, can be deduced analogously to the third step in the proof of Theorem 5. We have, by definition of $\bar{\beta}$,

$$(3.15) \quad \|\bar{\beta} - \beta^*\|_\infty = \|\Sigma^{-1} X^\top \varepsilon / n\|_\infty$$

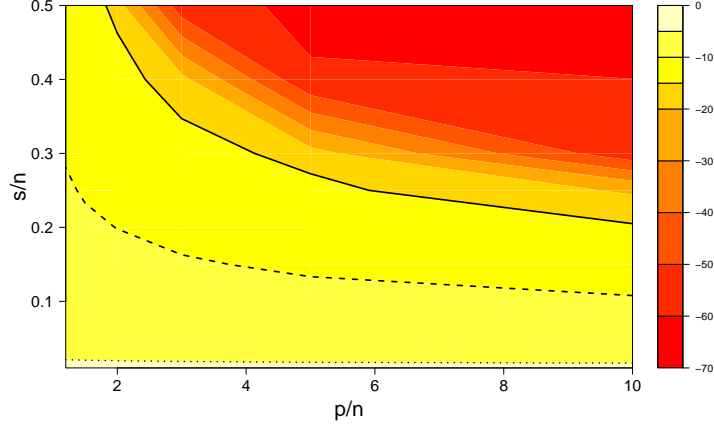


FIG 3. Empirical scalings of the quantity $\log_2(\tau^2(S))$ for Ens_+ in dependency of s/n and p/n , displayed in form of a contour plot. The lines indicates the level set for -15 (solid, $2^{-15} \approx 3 \cdot 10^{-5}$), -10 (dashed, $2^{-10} \approx 0.001$) and -5 (dotted, $2^{-5} \approx 0.03$).

When arguing as for (3.10), a lower bound on the square root of the smallest eigenvalue of Σ enters. However, if X is a square matrix, its smallest singular value is typically tiny so that a bound based on (3.15) is of little use. To get an idea of how that smallest singular value scales, one may look at certain classes of random matrices. Considering e.g. X whose rows are drawn i.i.d. from a sub-Gaussian distribution, recent results due to Rudelson and Vershynin [34, 35] imply that the smallest singular value scales as $O(n^{-1/2})$.

Sparsity of the NNLS solution. Using the decomposition technique underlying Theorem 5, it is argued in the sequel that the NNLS solution may be sufficiently sparse, which allows one to replace dependence on the smallest singular value of X by dependence on the smallest singular value of a tall rectangular submatrix. In case that the number of columns of that sub-matrix is proportionally small to the number of its rows, it is common in the literature on sparse recovery to assume that the smallest singular value of that matrix is lower bounded by a universal constant. More precisely, our argument evolves in the setup of Theorem 5 according to the following steps.

1. Lemma 1 states that the NNLS estimator can be obtained by least squares regression of y and a submatrix X_F , whose columns generate \mathcal{C}_F , the face of \mathcal{C} the observation vector y is projected on. We take $F = S \cup G$ as candidate for F , where S is the set of large coefficients of β^* and G , $|G| \leq (n - s)$, is the support of $\hat{\beta}^{(P1)}$ as defined in Lemma 2.
2. Provided $\Sigma_{FF}^{-1} X_F^\top y/n$ has only positive components, $\hat{\beta}_F = \Sigma_{FF}^{-1} X_F^\top y/n$, while $\hat{\beta}_{F^c} = 0$.
3. If the condition in 2.) is fulfilled, we have according to (3.15)

$$\|\hat{\beta}_F - \beta_F^*\|_\infty \leq \|\Sigma_{FF}^{-1} X_F^\top \varepsilon/n\|_\infty \leq \frac{2\sigma}{\sqrt{\phi_{\min}(F)}} \sqrt{\frac{2 \log p}{n}},$$

with probability at least $1 - 2/p$ as for (3.10), where $\phi_{\min}(F)$ is the smallest eigenvalue of Σ_{FF} .

With the same reasoning in the proof of Theorem 5, for the condition in 2.) to be fulfilled, it has to hold that

$$(3.16) \quad \beta_{\min}(S) > \frac{2\sigma}{\sqrt{\phi_{\min}(F)}} \sqrt{\frac{2 \log p}{n}}.$$

This may constitute a significant improvement over the corresponding condition on $\beta_{\min}(S)$ in Theorem 5 if $\{\phi_{\min}(F)\}^{1/2}$, the smallest singular value of X_F/\sqrt{n} , is not too small. As explained above, this assumption is not overly restrictive as long as the set F has cardinality significantly smaller than n , which is fulfilled only if it holds for both S and G as defined in 1). While S is assumed to have small cardinality throughout, bounding $|G|$ constitutes a major obstacle. Yet, the hypothesis that $|G|$ is small, is perfectly plausible in view of the strong bound on $\|\hat{\beta}_{S^c}\|_1$ in terms of $\tau^2(S)$. We conclude by stating the following result.

THEOREM 7. *Let the data-generating model be as in Theorem 5 and set $F = \{j : \hat{\beta}_j > 0\}$ and $\tilde{b} = 2\sigma \{\phi_{\min}(F)\}^{-1/2} \sqrt{2 \log(p)/n}$. If $\beta_{\min}(S) > \tilde{b}$, then*

$$S \subseteq F, \quad \|\hat{\beta}_S - \beta_S^*\|_\infty \leq \tilde{b}, \quad \|\hat{\beta}_{S^c} - \beta_{S^c}^*\|_\infty \leq b, \quad b = \max\{\tilde{b}, \|\beta_{S^c}^*\|_\infty\}.$$

with probability no less than $1 - 2/p$.

A second set of conditions to bound $\|\hat{\beta} - \beta^*\|_\infty$. So far, our reasoning has mainly been based on $\tau(S)$, which scales well for designs with a dense, positive correlation structure. On the other hand, $\tau(S)$ decays rapidly in p for several designs of interest. Take orthonormal design, i.e. $\Sigma = I_p$ as an example. It is not hard to verify that in this case $\tau(S) = \tau(s) = 1/\sqrt{p-s}$, yet it is well-known that sparse recovery by thresholding works well in this case [14]. For this reason, we introduce a second quantity that permits us to cover this and further designs.

DEFINITION 2. *For some fixed $S \subset \{1, \dots, p\}$ and $Z = \Pi_S^\perp X_{S^c}$, the quantity $\omega(S)$ is defined as*

$$(3.17) \quad \omega(S) = \min_{\emptyset \neq F \subseteq \{1, \dots, p-s\}} \min_{v \in \mathcal{V}(F)} \left\| \frac{1}{n} Z_F^\top Z_F v \right\|_\infty, \quad \mathcal{V}(F) = \{v \in \mathbb{R}_+^{|F|} : \|v\|_\infty = 1\}.$$

As compared to $\tau(S)$, $\omega(S)$ is obviously less handy since in general it cannot be evaluated numerically once S is fixed, because $\omega(S)$ involves minimization over all square sub-matrices of $\frac{1}{n} Z^\top Z$. Furthermore, while the geometric meaning is less transparent, it can be shown that $\omega(S)$ quantifies separation of the cones \mathcal{C}_S and \mathcal{C}_{S^c} as well. In Appendix F, the following properties are proved.

$$(3.18) \quad \omega(S) > 0 \Leftrightarrow \tau(S) > 0 \Leftrightarrow \mathcal{C}_S \text{ is a face of } \mathcal{C},$$

$$(3.19) \quad \omega(S) \leq 1, \text{ with equality if } \{X_j\}_{j \in S} \perp \{X_j\}_{j \in S^c} \text{ and } \frac{1}{n} X_{S^c}^\top X_{S^c} \succeq 0$$

$$(3.20) \quad \omega(S) \geq \min_{1 \leq j \leq (p-s)} \frac{1}{n} (Z^\top Z)_{jj} + \frac{1}{n} \sum_{k \neq j} \min\{(Z^\top Z)_{jk}, 0\},$$

The lower bound (3.20) is rather conservative. One can think of $\omega(S)$ being lower bounded by a positive constant as long as there are no large principal

submatrices of $\frac{1}{n}Z^\top Z$ with significantly negative off-diagonal entries.

For Theorem 8 below, we need in addition to the quantities in (3.4) the following constant, which is similar to the so-called *cumulative local coherence* used in [8], which specifically addresses the case where for a small number of pairs (j, k) , $|\sigma_{jk}| = \left| \frac{1}{n}X_j^\top X_k \right|$ is significant, while it is close to zero otherwise. We set

$$(3.21) \quad \mu_+(S) = \max_{j \in S} \sum_{k \in S^c} |\sigma_{jk}|.$$

THEOREM 8. *Let the data-generating model be as in Theorem 5. Set*

$$b = \frac{\|\beta_{S^c}^*\|_1 + 2\sigma\sqrt{\frac{2\log p}{n}}}{\omega(S)}, \quad \tilde{b} = (b + \|\beta_{S^c}^*\|_1) \mu_+(S) K(S) + \frac{2\sigma}{\sqrt{\phi_{\min}(S)}} \sqrt{\frac{2\log p}{n}}.$$

If $\beta_{\min}(S) > \tilde{b}$, then the NNLS estimator $\hat{\beta}$ has the following properties with probability no less than $1 - 4/p$

$$\|\hat{\beta}_{S^c}\|_\infty \leq b, \quad \|\hat{\beta}_S - \beta_S^*\|_\infty \leq \tilde{b}.$$

PROOF. The proof parallels that of Theorem 5. Only the differences in reasoning are given.

Step 1: The constant $\omega(S)$ gives rise to a bound on the ℓ_∞ -norm of $\hat{\beta}^{(P1)}$. In view of Lemma 1, there exists a set $F \subseteq \{1, \dots, p-s\}$ (we may assume $F \neq \emptyset$, otherwise $\hat{\beta}^{(P1)} = 0$) s.t. $\hat{\beta}_{F^c}^{(P1)} = 0$ and s.t.

$$\frac{1}{n}Z_F^\top Z_F \hat{\beta}_F^{(P1)} = \frac{1}{n}Z_F^\top (\xi + Z\beta_{S^c}^*),$$

which implies that

$$\begin{aligned} \left\| \frac{1}{n}Z_F^\top Z_F \hat{\beta}_F^{(P1)} \right\|_\infty &\leq A + \left\| \frac{1}{n}Z_F^\top Z_F \beta_{S^c}^* \right\|_\infty \leq A + \|\beta_{S^c}^*\|_1, \quad A = \left\| \frac{1}{n}Z_F^\top \xi \right\|_\infty, \\ \Rightarrow \min_{v \in \mathcal{V}(F)} \left\| \frac{1}{n}Z_F^\top Z_F v \right\|_\infty \|\hat{\beta}^{(P1)}\|_\infty &\leq A + \|\beta_{S^c}^*\|_1, \quad \mathcal{V}(F) = \{v \in \mathbb{R}_+^{|F|} : \|v\|_\infty = 1\}, \\ \Rightarrow \min_{\emptyset \neq F \subseteq \{1, \dots, p-s\}} \min_{v \in \mathcal{V}(F)} \left\| \frac{1}{n}Z_F^\top Z_F v \right\|_\infty \|\hat{\beta}^{(P1)}\|_\infty &\leq A + \|\beta_{S^c}^*\|_1, \\ \Rightarrow \omega(S) \|\hat{\beta}^{(P1)}\|_\infty &\leq A + \|\beta_{S^c}^*\|_1, \end{aligned}$$

where we have used Definition 2. We conclude that $\|\hat{\beta}^{(P1)}\|_\infty \leq (A + \|\beta_{S^c}^*\|_1)/\omega(S)$.

In Step 2, the bound (3.9) is changed as follows.

$$\|\Sigma_{SS}^{-1} \Sigma_{SS^c} (\hat{\beta}^{(P1)} - \beta_{S^c}^*)\|_\infty \stackrel{(3.4), (3.21)}{\leq} K(S) \mu_+(S) (\|\hat{\beta}^{(P1)}\|_\infty + \|\beta_{S^c}^*\|_1).$$

The remainder of the proof is along the lines of the proof of Theorem 5, *mutatis mutandis*. \square

Example: power decay. Let the entries of the Gram matrix Σ be given by $\sigma_{jk} = \rho^{|j-k|}$, $1 \leq j, k \leq p$, $0 \leq \rho < 1$. In general, Σ can be identified with a covariance matrix of a set of zero-mean, unit variance random variables $\{R_j\}_{j=1}^p$. Correspondingly, for any $S \subset \{1, \dots, p\}$, the matrix

$$(3.22) \quad \frac{1}{n}Z^\top Z = \frac{1}{n}X_{S^c}^\top (I - \Pi_S) X_{S^c} = \Sigma_{S^c S^c} - \Sigma_{S^c S} \Sigma_{SS}^{-1} \Sigma_{SS^c}$$

can be interpreted as the *conditional* covariance matrix of the random variables $\{R_j\}_{j \in S^c}$ conditional on $\{R_j\}_{j \in S}$. The power decay structure of Σ gives rise to a Markov random field in which the conditional covariances satisfy $\text{Cov}(R_k, R_l | \{R_j\}_{j \in S}) \geq 0$, $k, l \notin S$, with equality if S contains an index m such that $\min\{k, l\} < m < \max\{k, l\}$, see e.g. [36]. Hence all entries of $\frac{1}{n}Z^\top Z$ are non-negative, such that, using (3.20), $\omega(S) \geq \min_{1 \leq j \leq (p-s)} \frac{1}{n}(Z^\top Z)_{jj}$. A lower bound on the minimum diagonal entry is obtained by noting that

$$(3.23) \quad \frac{1}{n}(Z^\top Z)_{jj} = \text{Var}(R_j | \{R_k\}_{k \in S}) \geq \text{Var}(R_j | \{R_{j-1}, R_{j+1}\}) = \sigma_{jj} - \Sigma_{j\mathcal{N}}(\Sigma_{\mathcal{N}\mathcal{N}})^{-1}\Sigma_{\mathcal{N}j},$$

with $\mathcal{N} = \{j-1, j+1\}$ (we may exclude the cases $j=1$ and $j=p$, since the minimum is not attained there) and

$$\Sigma_{j\mathcal{N}} = [\rho \quad \rho], \quad \Sigma_{\mathcal{N}\mathcal{N}} = \begin{bmatrix} 1 & \rho^2 \\ \rho^2 & 1 \end{bmatrix}.$$

Explicit computation of the r.h.s. of (3.23) then yields that $\frac{1}{n}(Z^\top Z)_{jj} \geq 1 - \frac{2\rho^2}{1+\rho^2}$. Moreover, it is well-known [36] that the negative off-diagonal entries of the *inverse* of a covariance matrix are – up to a positive multiplicative constant – equal to the conditional covariances after conditioning on all remaining variables, i.e. for $j \neq k$, $(\Sigma^{-1})_{jk} \propto -\text{Cov}(R_j, R_k | \{R_l\}_{l \notin \{j,k\}})$. In view of the specific Markov random field structure, $\text{Cov}(R_j, R_k | \{R_l\}_{l \notin \{j,k\}}) = 0$ whenever $|j-k| > 1$. It thus follows that, independent of S , Σ_{SS}^{-1} has at most two non-zero off-diagonal entries per row. Hence, $K(S)$ and $\phi_{\min}(S)$ as defined in (3.4) are necessarily upper and lower bounded by constants depending on ρ only, but not on s . By the geometric series formula, $\mu_+(S) \leq \frac{\rho}{1-\rho}$. In total, by invoking Theorem 8 with $\|\beta_{S^c}^*\|_1 = 0$, one obtains an ℓ_∞ -error of the right order

$$\|\hat{\beta} - \beta^*\|_\infty \leq C_\rho \sigma \sqrt{\log(p)/n},$$

for a constant $C_\rho > 0$ depending on ρ only.

Support recovery by thresholding. It follows immediately from Theorems 7 and 8 that the set S of large coefficients can be recovered by hard thresholding. Let $t \geq 0$ be a threshold. Then the hard-thresholded NNLS estimator is defined by

$$(3.24) \quad \hat{\beta}_j(t) = \begin{cases} \hat{\beta}_j, & \hat{\beta}_j > t, \\ 0, & \text{otherwise, } j = 1, \dots, p. \end{cases}$$

Let us further define $\hat{S}(t) = \{j : \hat{\beta}_j > 0\}$. In the setting of Theorems 7 or 8, if $t > b$ and if $\beta_{\min}(S) > b + \tilde{b}$, one has that $S = \hat{S}(t)$ with the stated probabilities. Choosing the threshold t according to the bounds of Theorems 7 and 8 is impractical, since it involves dependence on constants that are not accessible. In the following, we suggest to use a simple data-driven procedure proposed in [22] to be used in conjunction with marginal regression, which avoids direct specification of t . Instead, one attempts to estimate s . To simplify the exposition, we shall assume for the remainder of the paragraph that $\|\beta_{S^c}^*\|_1 = 0$.

A crucial observation in [22] is that if there are statistics giving rise to a ranking $(r_j)_{j=1}^p$ of the predictors $\{X_j\}_{j=1}^p$ so that $r_j \leq s$ for all $j \in S$, then it is sufficient for support recovery to estimate the support size s and select all predictors of rank no larger than s . It is a consequence of Theorems 7 and 8 that

if $\beta_{\min}(S)$ is large enough, the NNLS estimator $\hat{\beta}$ gives rise to such a ranking by setting

$$(3.25) \quad r_j = k \Leftrightarrow \hat{\beta}_j = \hat{\beta}_{(k)}, j = 1, \dots, p, \quad \hat{\beta}_{(1)} \geq \hat{\beta}_{(2)} \geq \dots \geq \hat{\beta}_{(p)}.$$

In [22], where Gaussian noise is assumed, the following estimate \hat{s} for s is suggested. In the sequel, denote by $\vartheta^2 = \mathbf{E}[\varepsilon^2]$ the variance of ε .

$$(3.26) \quad \hat{s} = \max \left\{ 0 \leq k \leq (p-1) : \delta(k) \geq \vartheta \sqrt{2 \log n} \right\} + 1,$$

$$(3.27) \quad \delta(k) = \|(\Pi(k+1) - \Pi(k))y\|_2, \quad k = 0, \dots, (p-1),$$

where $\Pi(k)$ denotes the orthogonal projection on the subspace spanned by the variables with ranks no larger than k and $\Pi(0) = 0$. Note that the estimate \hat{s} in (3.26) depends on the noise variance ϑ^2 , which is unknown in general. However, one may replace it by a simple plug-in estimate resulting from the NNLS fit, provided its ℓ_2 -prediction error $\frac{1}{n} \|X\beta^* - X\hat{\beta}\|_2^2$ is small enough. More specifically, we have the following theorem that hinges on a result in [22].

THEOREM 9. *Let the data-generating model be as in Theorem 5 with $\|\beta_{S^c}^*\|_1 = 0$. Let b, \tilde{b} be as in Theorem 7 or Theorem 8. If $\beta_{\min}(S) > b + \tilde{b}$ and*

$$\frac{\vartheta \sqrt{\log n}}{\min_{j \in S} \|(\Pi_S - \Pi_{S \setminus j})X_j \beta_j^*\|_2} \rightarrow 0 \quad \text{as } n \rightarrow \infty,$$

and if there exists $c, C > 0$ such that, with probability tending to one as $n \rightarrow \infty$,

$$(3.28) \quad c\vartheta \leq \hat{\vartheta} \leq C\vartheta, \quad \text{where } \hat{\vartheta}^2 = \|y - X\hat{\beta}\|_2^2/n,$$

then, $\hat{S} = S$ with probability tending to one, where $\hat{S} = \{j : r_j \leq \hat{s}\}$, with $\{r_j\}_{j=1}^p$ as in (3.25) and \hat{s} is the estimate of s according to (3.26), with ϑ replaced by $\hat{\vartheta}$.

We point out again that the strategy for (implicitly) selecting the threshold according to Theorem 9 does not require the specification of any parameter by the user. The output \hat{S} results from a *single* NNLS fit plus repeated evaluation of (3.27), with ϑ^2 replaced by the plug-in estimator (3.28), until the stopping criterion in (3.26) is reached, which can be done efficiently by updating QR decompositions.

Finally, we point out that subsequent to thresholding, it is beneficial to recompute the NNLS solution using data $(y, X_{\hat{S}})$ only, because the removal of superfluous variables leads to a more accurate estimation of the support coefficients.

3.7. Comparison of NNLS and the non-negative lasso. In the literature on high-dimensional statistical models and sparse recovery, ℓ_1 -regularization has received most attention, see the retrospective [42], and is often propagated as the method of choice due to ease of computation and strong theoretical guarantees. Similar guarantees for certain designs that are, roughly speaking, characterized by a positive correlation structure, have been established for NNLS in the preceding sections. In the present subsection, we enumerate several advantages of NNLS over ℓ_1 -regularization, some of which are confirmed by numerical studies discussed in Section 4.

The non-negative lasso. Consider the non-negative lasso problem

$$(3.29) \quad \min_{\beta \succeq 0} \frac{1}{n} \|y - X\beta\|_2^2 + \lambda \mathbf{1}^\top \beta, \quad \lambda > 0,$$

with minimizer denoted by $\widehat{\beta}^{\ell_1, \succeq}$. In the remainder of the paragraph, we study $\widehat{\beta}^{\ell_1, \succeq}$ from the point of view of variable selection under a non-negative version of the 'irrepresentable condition' which has been shown to be a sufficient and essentially necessary condition for support recovery of the lasso [32, 47, 53].

DEFINITION 3. *Let $S \subset \{1, \dots, p\}$ be given. The non-negative irrepresentable constant is defined as the smallest value $\gamma(S) \in [0, 1]$ such that*

$$(3.30) \quad X_{S^c}^\top X_S (X_S^\top X_S)^{-1} \mathbf{1} \preceq (1 - \gamma(S)) \mathbf{1}.$$

Similarly to the constant $\tau(S)$ used in our analysis of NNLS, the irrepresentable constant also quantifies separation between support and off-support, with the important difference that the separating functional is affine instead of linear. In fact, we may equivalently express (3.30) as

$$X_{S^c}^\top w + b \mathbf{1} \succeq \gamma(S) \mathbf{1}, \quad X_S^\top w + b \mathbf{1} = 0, \quad w = -X_S (X_S^\top X_S)^{-1} \mathbf{1}, \quad b = 1.$$

By straightforward modifications of techniques employed in [47], a positive lower bound on $\gamma(S)$ gives rise to the following properties of $\widehat{\beta}^{\ell_1, \succeq}$ as sketched in Appendix H.

THEOREM 10. *Consider the data-generating model $y = X\beta^* + \varepsilon$, where ε has i.i.d. zero-mean sub-Gaussian entries with parameter σ , $\beta_S^* \succeq \beta_{\min}(S) > 0$ and $\beta_{S^c}^* = 0$. If*

$$(3.31) \quad \lambda > \frac{2\lambda_0}{\gamma(S)}, \quad \lambda_0 = 2\sigma \sqrt{\frac{2 \log p}{n}}, \quad \text{and } \beta_{\min}(S) > \tilde{b}, \quad \tilde{b} = \lambda \|\Sigma_{SS}^{-1} \mathbf{1}\|_\infty + \frac{\lambda_0}{\sqrt{\phi_{\min}(S)}},$$

it holds that $\|\widehat{\beta}_S^{\ell_1, \succeq} - \beta_S^\|_\infty \leq \tilde{b}$ and that $\widehat{\beta}_{S^c}^{\ell_1, \succeq} = 0$ with probability at least $1 - 2/p$.*

It further follows from the analysis in [47] that a positive lower bound on $\gamma(S)$ is also a necessary condition for support recovery. Moreover, there is a striking resemblance of the result (3.31) and that of Theorem 5, with $\tau^2(S)$ playing a similar role as $\gamma(S)$ and structurally roughly the same condition on $\beta_{\min}(S)$, noting that $\|\Sigma_{SS}^{-1} \mathbf{1}\|_\infty$ is related to the constant $K(S)$ defined in (3.4).

From (3.31) one *cannot* deduce that the non-negative lasso attains the optimal ℓ_∞ -rate for estimating β^* , because $\gamma(S)$ may be decreasing in s and $\|\Sigma_{SS}^{-1} \mathbf{1}\|_\infty$ may be of order $O(\sqrt{s})$. The assumption that $\gamma(S)$ is uniformly bounded away from zero is considered to be rather restrictive [33]. On the other hand, under a restricted eigenvalue condition [3], which is closely related to Condition 2 of the present paper and which applies much more broadly than the 'strong irrepresentable condition' of [53], $\|\widehat{\beta}^{\ell_1, \succeq} - \beta^*\|_2$ is of the order $O(\sqrt{s \log(p)/n})$ [3], which is in general not improvable apart from the log factor. However, it is no longer guaranteed that $\widehat{\beta}_{S^c}^{\ell_1, \succeq} = 0$, so that subsequent hard thresholding

of $\widehat{\beta}^{\ell_1, \geq}$ has been proposed as remedy [33, 54]. The ℓ_2 -bound requires a sub-optimal condition on $\beta_{\min}(S)$ for thresholding to identify the support S . Optimal rates in sup-norm of the order $O(\sqrt{\log(p)/n})$ are derived in [9, 30] under a ‘mutual incoherence’ condition which, however, in general requires the recoverable sparsity level s to be of the order $o(\sqrt{n})$. The fact that ℓ_1 -regularization behaves suboptimally with regard to its ℓ_∞ -error, which is eventually decisive when one is interested in accurate feature selection, is stressed in [52]. In the cited references, non-negativity constraints do not appear; however, apart from possible changes in constants, we do not see how these constraints could lead to a substantially different theory.

NNLS vs. the non-negative lasso: pros and cons. To sum up, we list advantages and disadvantages of NNLS and the non-negative lasso, thereby providing some guidance on when to use which approach in practice. While NNLS can formally be seen as a special case of the non-negative lasso as $\lambda \rightarrow 0$, we always think of the latter as applied with a significant amount of regularization (i.e. it is implicitly assumed that $\lambda \geq \lambda_0$, with λ_0 as in (3.31)).

- A drawback of NNLS is that its success for high-dimensional linear models is coupled with conditions on the design, the half-space condition (\mathcal{H}) being a minimum requirement. If these conditions are not met, NNLS is hopelessly prone to overfitting. A noted advantage of the non-negative lasso is that it performs well for a broader class of designs.
- There are designs for which NNLS achieves a better performance for estimating β^* in sup-norm and hence yields better performance with regard to feature selection via thresholding. On the other hand, as far as the ℓ_2 -error for β^* or the prediction error is concerned, one cannot expect a pronounced difference of the two approaches.
- From the point of view of a practitioner, NNLS possesses an important advantage over the non-negative lasso: it can be applied directly, without the need to specify a regularization parameter. As asserted by Theorem 9, the threshold can be chosen in an entirely data-driven, computationally inexpensive manner. This strongly contrasts with the use of regularization-based methods which usually involves cross-validation in conjunction with a grid search for the regularization parameter(s).

4. Illustrations. We conclude by presenting experimental results illustrating important aspects discussed in the paper.

4.1. Deconvolution of spike trains. We consider a positive spike-deconvolution model as in [28], which is of importance in various fields of applications. It is assumed that the underlying signal f , which is a function on $[a, b]$, is of the form

$$f(u) = \sum_{k=1}^s \beta_k^* \phi_k(u), \quad u \in [a, b],$$

with $\phi_k(\cdot) = \phi(\cdot - \mu_k)$, $k = 1, \dots, s$, where $\phi \geq 0$ is known as *point-spread function (PSF)* and the μ_k ’s define the locations of the spikes contained in $[a, b]$. The amplitudes $\{\beta_k^*\}_{k=1}^s$ are assumed to be positive. Assuming further that the PSF is known, the problem consists of determining the positions as well as the amplitudes of the spikes from n (potentially noisy) samples of the

underlying signal f . As demonstrated below, NNLS can be a first step towards deconvolution. The idea is to construct a design matrix of the form $X = (\phi_j(u_i))$, where $\phi_j = \phi(\cdot - m_j)$ for candidate positions $\{m_j\}_{j=1}^p$ placed densely in $[a, b]$ and $\{u_i\}_{i=1}^n \subset [a, b]$ are the points at which the signal is sampled. Under an additive noise model with zero-mean sub-Gaussian noise ε , i.e.

$$y_i = \sum_{k=1}^s \beta_k^* \phi_k(u_i) + \varepsilon_i, \quad i = 1, \dots, n,$$

and if X has the self-regularizing property (2.5), cf. Section 2.4, it follows immediately from Theorem 3 that the ℓ_2 -prediction error of NNLS is nicely bounded in the sense that

$$(4.1) \quad \frac{1}{n} \|f - X\hat{\beta}\|_2^2 \leq \mathcal{E}^* + C \sqrt{\frac{\log p}{n}}, \quad \{f_i = f(u_i)\}_{i=1}^n,$$

holds with high probability, where $\mathcal{E}^* = \min_{\beta \geq 0} \frac{1}{n} \|f - X\beta\|_2^2$. Note that it is not realistic to assume that $\{\mu_k\}_{k=1}^p \subset \{m_j\}_{j=1}^p$, i.e. that the linear model is correctly specified, albeit we may think of \mathcal{E}^* being negligible as long as the $\{m_j\}_{j=1}^p$ are placed densely enough. This means that NNLS may be suitable for de-noising. Furthermore, the bound (4.1) implies that $\hat{\beta}$ must have large components for those columns of X corresponding to locations near the locations $\{\mu_k\}_{k=1}^s$ of the spikes, which can then be estimated accurately by applying a simple form of post-processing as discussed in [39].

Figure 1 displays the outcome of an example, in which the design matrix is specified correctly so that \mathcal{E}^* equals zero. The underlying signal is composed of five spikes of amplitudes between 0.2 and 0.7 convolved with a Gaussian function. The design matrix $X = (\phi_j(u_i))$ contains evaluations of $p = 200$ Gaussians $\{\phi_j\}_{j=1}^p$ at $n = 100$ points $\{u_i\}_{i=1}^n$, where both the centers of the $\{\phi_j\}$ as well as the $\{u_i\}_{i=1}^n$ are equi-spaced in the unit interval. The standard deviation of the Gaussians is chosen such that it is roughly twice the spacing of the $\{u_i\}$. At this point, it is important to note that the larger the standard deviations of the Gaussians, the larger becomes the constant τ_0 , cf. (2.5). Additive Gaussian noise with standard deviation 0.09 is used.

From the left panel of Figure 4, we conclude that over-fitting scarcely occurs, the only visible exception being the region between 0.5 and 0.6. The right panel displays the coefficient vector $\hat{\beta}$, which is remarkably sparse and concentrated near (in some cases precisely at) the positions of the underlying spikes.

4.2. Sparse recovery: comparison of the non-negative lasso and NNLS. The present subsection illustrates the excellent performance of NNLS with respect to sparse recovery by thresholding.

Setup. We randomly generate data $y = X\beta^* + \varepsilon$, where ε has i.i.d. standard Gaussian entries. We consider two choices for the design X . For one set of experiments, the rows of X are drawn i.i.d. from a Gaussian distribution whose covariance matrix has the power decay structure of the example following Theorem 8 with parameter $\rho = 0.7$. For the second set, we pick a representative of the class Ens_+ (3.13), drawing each entry of X uniformly from $[0, 1]$ and re-scaling such that the population Gram matrix has equi-correlation structure with $\rho = 3/4$, precisely as for the numerical results regarding the scaling

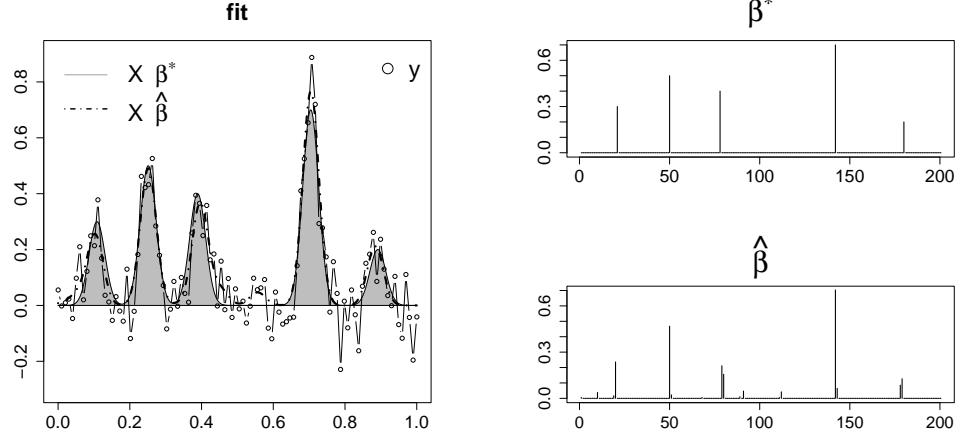


FIG 4. Left panel: Data as described in the text. The grey area represents $X\beta^*$, a linear combination of five Gaussians. The dashed line represents the NNLS fit $X\hat{\beta}$. Right panel: True coefficients $\{\beta_j^*\}_{j=1}^p$ (top) and NNLS coefficients $\{\hat{\beta}_j\}_{j=1}^p$ (bottom).

of $\tau^2(S)$ in Section 3.5. The target β^* is generated by selecting its support S uniformly at random ($\beta_{S^c}^* = 0$) and then setting $\beta_j^* = b \cdot \beta_{\min}(S)(1 + U_j)$, $j \in S$, with $\beta_{\min}(S) = C_\rho \sqrt{2 \log(p)/n}$, where C_ρ is obtained by evaluating the constants appearing in the condition on $\beta_{\min}(S)$ in Theorems 7 and 8 based on the underlying population Gram matrices; the $\{U_j\}_{j \in S}$ are drawn i.i.d. uniformly from $[0, 1]$, and b is a parameter controlling the signal strength. The experiments can be divided into two parts. In the first part, the parameter b is kept fixed while the aspect ratio p/n of X and the fraction of sparsity s/n vary. In the second part, s/n is fixed to 0.2, while p/n and b vary. When not fixed, $s/n \in \{0.05, 0.1, 0.15, 0.2, 0.25, 0.3\}$. The grid used for b is chosen specific to the designs, calibrated such that the sparse recovery problems are sufficiently challenging. For the design from Ens_+ , $p/n \in \{2, 3, 5, 10\}$, whereas for power decay $p/n \in \{1.5, 2, 2.5, 3, 3.5, 4\}$, for reasons that will become clear from the results. Each configuration is replicated 100 times for $n = 500$.

Comparison. Across these runs, we compare the probability of ‘success’ of thresholded NNLS (tNNLS), non-negative lasso ($\text{NN}\ell_1$) as defined in (3.29), thresholded non-negative lasso ($\text{tNN}\ell_1$) and orthogonal matching pursuit (OMP, [43, 51]). We also compare against the ordinary lasso (2.9); since its performance is mostly nearly equal, partially considerably worse than that of its non-negative counterpart (see the right panel of Figure 5 for an example), the results are not shown in the remaining plots for the sake of better readability. ‘Success’ is defined as follows. For tNNLS, we have ‘success’ if $\min_{j \in S} \hat{\beta}_j > \max_{j \in S^c} \hat{\beta}_j$, i.e. there exists a threshold that permits support recovery. For $\text{NN}\ell_1$, we set $\hat{\lambda} = 2\|X^\top \varepsilon/n\|_\infty$, which is the empirical counterpart to $\lambda_0 = 2\sqrt{2 \log(p)/n}$, the choice for the regularization parameter advocated in [45] to achieve the optimal rate for the estimation of β^* in the ℓ_2 -norm, and compute the whole set of solutions $\{\hat{\beta}(\lambda), \lambda \geq \hat{\lambda}\}$ using the non-negative lasso modification of LARS [21] and check whether the sparsity pattern of *one* of these solutions recovers S . For $\text{tNN}\ell_1$, we implement a strategy that has essentially been proposed in [33] as a remedy for the tendency of the lasso to over-select, assigning small non-zero

coefficients to elements from S^c . On the other hand, the lasso yields an estimate close to β^* in the ℓ_2 -norm, such that subsequent thresholding may be an effective strategy to get rid of false positive selections. In our experiments, we inspect the set of non-negative lasso solutions $\{\hat{\beta}(\lambda) : \lambda \in [\lambda_0 \wedge \hat{\lambda}, \lambda_0 \vee \hat{\lambda}]\}$ and check whether $\min_{j \in S} \hat{\beta}_j(\lambda) > \max_{j \in S^c} \hat{\beta}_j(\lambda)$ holds for *one* of these solutions; with the range chosen for λ , we aim at having solutions that approximate β^* well in ℓ_2 -norm. We believe that this procedure is more reliable than fixing λ to one specific value known to give the optimal rate in theory. Note that, when comparing tNNLS and tNN ℓ_1 , the lasso is given an advantage, since we optimize over a range of solutions. Lastly, for OMP, we check whether the support S is recovered in the first s steps.

Results. The approaches NN ℓ_1 and OMP are not competitive – both work only with rather moderate levels of sparsity, with a breakdown at $s/n = 0.15$ for power decay as displayed in the left panel of Figure 5. For equi-correlation-like design, the results are even worse. This is in accordance with the literature where thresholding is proposed as remedy [33, 52, 54]. Yet, for a wide range of configurations, tNNLS visibly outperforms tNN ℓ_1 , a notable exception being power decay with larger values for p/n (see Figure 6). This is in contrast to the design from Ens $_+$, where even $p/n = 10$ can be handled. In fact, power decay is noticeably different from equi-correlation-like design with regard to the scaling of the constant $\tau^2(S)$. One can show that for the population Gram matrix, it holds that $\tau^2(S) \leq 2(1 - \rho)^{-1}(p - s)^{-1} = O((p - s)^{-1})$ uniformly in S . As a result, it is not helpful to apply Theorem 5. On the other hand, Theorem 8 involves the constant $\omega(S)$ whose scaling for random designs is not clear. This issue requires future research, which could considerably improve the understanding of NNLS in a high-dimensional setting.

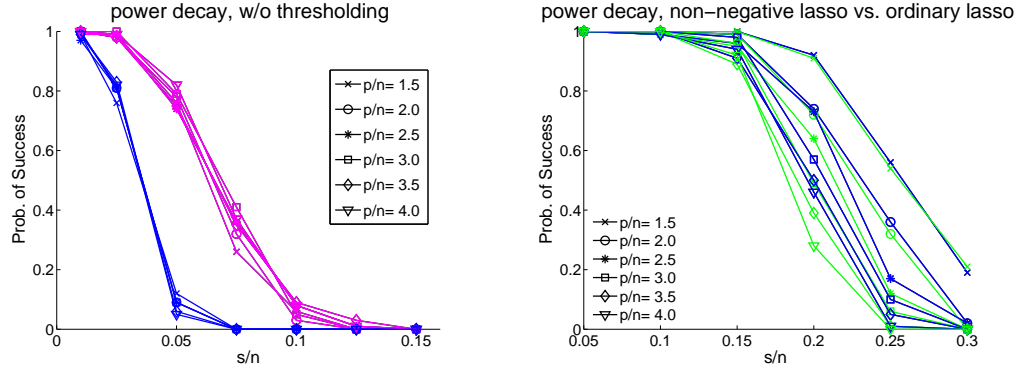


FIG 5. Left: Probability of success of the non-negative lasso **without** thresholding (blue) and orthogonal matching pursuit (magenta). Right: Probability of success of the thresholded non-negative lasso (blue) and thresholded ordinary lasso (green).

Data-driven selection of the threshold. In the experiments of the previous paragraph, an explicit choice of the threshold has been avoided. Instead, we have confined us to examine whether there is a threshold permitting support recovery, given full information about the underlying S , which is not available in practice. On the other hand, we have outlined a scheme for an implicit data-driven choice of the threshold, which is consistent as asserted by Theorem 9. We here report results of an experiment that essentially confirms the finding of

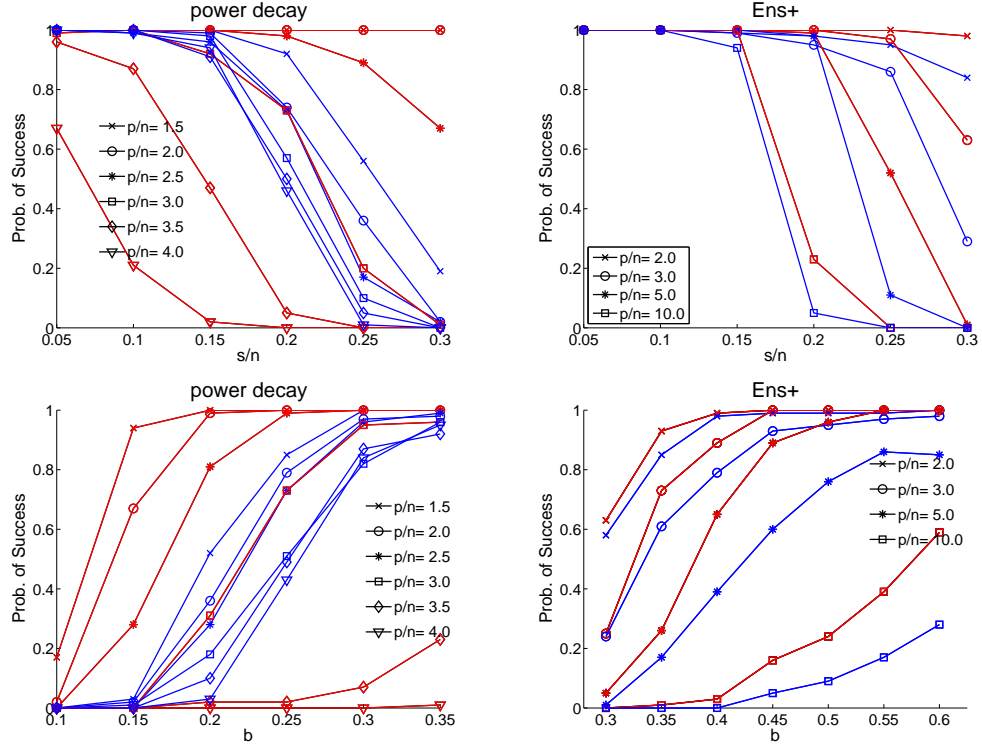


FIG 6. Comparison of thresholded NNLS (red) and thresholded non-negative lasso (blue). Top: Probability of success for the experiments with constant b , while s/n (abscissa) and p/n (symbols) vary. Bottom: Probability of success for the experiments with constant s/n , while b (abscissa) and p/n (symbols) vary.

Theorem 9. The experimental setup follows that of the previous paragraph. We take random design with i.i.d. uniformly distributed entries. Taking $n = 500$, The range for p/n remains unchanged, while $s/n \in \{0.01, 0.025, 0.05, 0.1, 0.2\}$, excluding critically high values such as 0.25 and 0.3; the generation of the non-zero entries of β^* remains unchanged as well (the signal strength parameter b is kept fixed). The average number of false positive selections over 100 replications in dependency of s/n and p/n is displayed in Figure 7. The results are rather

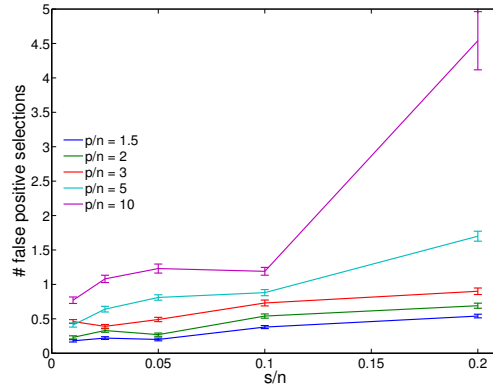


FIG 7. Average number of false positive selections when using the estimator of s of Theorem 9. Note the extremely low percentage of false positive selections when compared to s or p ($n = 500$, i.e. $p \in \{750, 1000, 1500, 2500, 5000\}$).

promising: false positive selections occur rarely, the absolute number ranging from less than one in the majority to a maximum of roughly five in the most difficult setting. Note that even in this extreme case, five false positives are only one percent of $p = 5000$ and only five percent of $s = 100$. Moreover, the situation is even better as far as false negatives are concerned. Only for $s/n = 0.2$ and $p/n \geq 5$, false negatives occur at all (on average 0.02 and 2.25, respectively).

Acknowledgements. We would like to thank Mike Davies, Rolf Schneider, Jared Tanner and Roman Vershynin for valuable discussions.

APPENDIX A: SUB-GAUSSIAN RANDOM VARIABLES

A random variable Z is called sub-Gaussian if there exists a positive constant K such that $\mathbf{E}[|Z|^q]^{1/q} \leq K\sqrt{q}$. The smallest such K is called the sub-Gaussian norm $\|Z\|_{\psi_2}$ of Z . If $\mathbf{E}[Z] = 0$, which shall be assumed for the remainder of this paragraph, then the moment-generating function of Z satisfies $\mathbf{E}[\exp(tZ)] \leq \exp(-t^2/(2\sigma^2))$ for a parameter $\sigma > 0$ which is related to $\|Z\|_{\psi_2}$ by a multiplicative constant, cf. [46]. It follows that if Z_1, \dots, Z_n are i.i.d. copies of Z and $v \in \mathbb{R}^n$, then $\sum_{i=1}^n v_i Z_i$ is sub-Gaussian with parameter $\|v\|_2^2 \sigma^2$. We have the well-known tail bound

$$(A.1) \quad \mathbf{P}(|Z| > z) \leq 2 \exp\left(-\frac{z^2}{2\sigma^2}\right), \quad z \geq 0.$$

Combining the previous two facts and using a union bound, with $\mathbf{Z} = (Z_1, \dots, Z_n)^\top$, it follows that for any collection of vectors $v_j \in \mathbb{R}^n$, $j = 1, \dots, p$,

$$(A.2) \quad \mathbf{P}\left(\max_{1 \leq j \leq p} |v_j^\top \mathbf{Z}| > \sigma \max_{1 \leq j \leq p} \|v_j\|_2 \sqrt{2 \log p} + \sigma z\right) \leq 2 \exp\left(-\frac{1}{2} z^2\right), \quad z \geq 0.$$

APPENDIX B: PROOF OF THEOREM 2

The proof relies on the following three auxiliary results.

Concentration of measure of Lipschitz functions of Gaussian random vectors.

THEOREM B. 1. (e.g. [46], Proposition 34)

Let f be a real-valued Lipschitz function on \mathbb{R}^n with Lipschitz constant L . Let g be a standard Gaussian random vector in \mathbb{R}^n . Then for every $z \geq 0$, it holds that

$$\mathbf{P}(f(g) - \mathbf{E}[f(g)] \geq z) \leq \exp(-z^2/(2L^2)), \quad \mathbf{P}(\mathbf{E}[f(g)] - f(g) \geq z) \leq \exp(-z^2/(2L^2)).$$

Concentration of extreme singular values of Gaussian random matrices. Denote by $s_{\min}(X)$ and $s_{\max}(X)$ the minimum and maximum singular value of a matrix X .

THEOREM B. 2. (e.g. [46], Corollary 35)

Let X be an $n \times s$ matrix whose entries are independent standard normal variables. Then for every $z \geq 0$, each of the following two events hold with probability at least $1 - \exp(-z^2/2)$:

$$s_{\min}(X) \geq \sqrt{n} - \sqrt{s} - z, \quad s_{\max}(X) \leq \sqrt{n} + \sqrt{s} + z.$$

A property of the convex hull of Gaussian vectors. The following result can be seen as a non-symmetric analog of a result of [24].

THEOREM B. 3. Let X_1, \dots, X_p be random n -dimensional standard Gaussian vectors. Denote their convex hull by \mathcal{K} . Then there exists constants $C_1 > 2, C_2, c > 0$ such that for all $p/n > C_1$, it holds that

$$\mathcal{K} \supset C_2 \min\{\sqrt{n}, \sqrt{\log(p/n)}\} B_2^n, \quad B_2^n = \{x \in \mathbb{R}^n : \|x\|_2 \leq 1\}.$$

with probability at least $1 - 2 \exp(-cn)$.

This result can be proved by straightforward modifications of the proof of a closely related result in [23]. In [23], the only difference is that $\{X_1, \dots, X_p\}$ are drawn according to the uniform distribution on a Euclidean ball.

Proof of Theorem 2. Let $\delta \in (0, 1)$. The event

$$E_1 = \{m_n(1 - \delta)\sqrt{n} \leq \|\varepsilon\|_2 \leq (1 + \delta)\sqrt{n}\}, \quad m_n = \sqrt{n/(n+1)}.$$

holds with probability at least $1 - 2\exp(-\delta^2 n/2)$. This follows from Theorem B.1, noting that $n/\sqrt{n+1} \leq \mathbf{E}[\|\varepsilon\|_2] \leq \sqrt{n}$ for all $n \geq 1$. Conditional on E_1 , for any $\beta \in \mathbb{R}^p$ such that $\|X\beta\|_2 \leq m_n(1 - \delta)\sqrt{n}/2$, the triangle inequality implies that

$$\|\varepsilon - X\beta\|_2 \geq m_n(1 - \delta)\sqrt{n}/2 \implies \frac{1}{n}\|\varepsilon - X\beta\|_2^2 \geq m_n^2(1 - \delta)^2/4.$$

In the sequel, it will be shown that one can find a numerical constant $C_0 > 2$ such that if $p/n > C_0$, it holds that

$$(B.1) \quad \min_{\beta \geq 0} \frac{1}{n}\|\varepsilon - X\hat{\beta}\|_2^2 < m_n^2(1 - \delta)^2/4,$$

with high probability, implying that $\frac{1}{n}\|X\hat{\beta}\|_2^2 > m_n(1 - \delta)^2/4 = \Omega(1)$, as to be shown. In order to show (B.1), the NNLS objective is decomposed as follows.

$$(B.2) \quad \frac{1}{n}\|\varepsilon - X\hat{\beta}\|_2^2 = \frac{1}{n} \left((\zeta - v^\top \hat{\beta})^2 + \|\xi - U\hat{\beta}\|_2^2 \right),$$

where we have decomposed ε as $\varepsilon = \begin{pmatrix} \zeta \\ \xi \end{pmatrix}$, with ζ denoting the first entry of ε .

Let \mathcal{K} denote the convex hull generated by the columns of U and let $\nu = n - 1$. By Theorem B.3, for $p/\nu > C_1$ and for some constant $C_2 > 0$, the event

$$E_2 = \{\mathcal{K} \supset C_2 r_{\nu,p} B_2^\nu\}, \quad r_{\nu,p} = \min\{\sqrt{\nu}, \sqrt{\log(p/\nu)}\}$$

holds with probability at least $1 - 2\exp(-c\nu)$. Hence, conditional on E_1 and E_2 , there exists $\tilde{\beta} \in \mathbb{R}_+^p$ having no more than ν non-zero entries so that

$$(B.3) \quad \xi = U\tilde{\beta} \quad \text{and} \quad \mathbf{1}^\top \tilde{\beta} \leq (1 + \delta)\sqrt{n} r_{\nu,p}^{-1} C_2^{-1}.$$

Moreover, it will be shown that there exists $C_3 > 0$ so that $\|\tilde{\beta}\|_2 \leq C_3$. Let U' of dimension $\nu \times \nu$ be the sub-matrix of U that is obtained by extracting the columns of U corresponding to the non-zero entries of $\tilde{\beta}$; accordingly, define β' as the corresponding sub-vector of $\tilde{\beta}$. Let further $J = \{j : \beta'_j \geq \frac{4C_4}{\sqrt{\nu}}\}$, where $C_4 > 0$ is chosen such that $\mathbf{1}^\top \tilde{\beta} \leq C_4\sqrt{\nu}$. Note that $|J| \leq \nu/4$. We have that

$$(B.4) \quad \|\xi\|_2 = \|U\tilde{\beta}\|_2 = \|U'\beta'\|_2 \geq \|U'_J\beta'_J\|_2 - \|U'_{J^c}\beta'_{J^c}\|_2 \geq s_{\min}(U'_J)\|\beta'_J\|_2 - s_{\max}(U')\|\beta'_{J^c}\|_2.$$

Conditional on E_2 , the event

$$E_3 = \{s_{\min}(U'_J) \geq \frac{1}{4}\sqrt{\nu}\} \cap \{s_{\max}(U') \leq \frac{9}{4}\sqrt{\nu}\},$$

holds with probability at least $1 - 2\exp(-\nu/32)$ by twofold application of Theorem B.2 with $z = \sqrt{\nu}/4$. Further note that by construction, $\|\beta'_{J^c}\|_2 \leq 4C_4$.

Consequently, if $\|\beta'_J\|_2$ were growing with n , the left hand side of (B.4) were of larger order than $O(\sqrt{n})$, contradicting $\|\xi\|_2 \leq (1 + \delta)\sqrt{n}$ conditional on E_1 . We conclude that conditional on E_1 , E_2 and E_3 , $\|\tilde{\beta}\|_2 \leq C_3$, $C_3 > 0$. Equipped with these intermediate results, we are in position to upper bound (B.2). Since $\tilde{\beta}$ is feasible for the NNLS problem, we have

$$\frac{1}{n}\|\varepsilon - X\hat{\beta}\|_2^2 \leq \frac{1}{n}\left((\zeta - v^\top \tilde{\beta})^2 + \|\xi - U\tilde{\beta}\|_2^2\right) \leq \frac{2}{n}\zeta^2 + \frac{2}{n}(v^\top \tilde{\beta})^2.$$

Since the entries of v are i.i.d. zero-truncated Gaussian random variables having mean $\sqrt{\frac{2}{\pi}}$, we may decompose $v = \sqrt{\frac{2}{\pi}}\mathbf{1} + \omega$, where $\omega = v - \sqrt{\frac{2}{\pi}}\mathbf{1}$ has i.i.d. zero-mean sub-Gaussian entries. Conditional on E_1 to E_3 , the tail bound (A.1) yields that

$$\mathbf{P}(E_4) \leq \exp(-c'nr_{\nu,p}^{-2}), \quad E_4 = \left\{v^\top \tilde{\beta} \geq \sqrt{\frac{2}{\pi}}(\mathbf{1}^\top \tilde{\beta}) + (1 + \delta)\sqrt{n} C_3 C_2^{-1} r_{\nu,p}^{-1}\right\},$$

for some constant $c' > 0$, cf. (B.3). Recall that according to (B.1), it suffices to show that

$$\frac{2}{n}\|\zeta\|_2^2 + \frac{2}{n}(v^\top \tilde{\beta})^2 < m_n^2(1 - \delta)^2/4.$$

The first summand on the l.h.s. of the inequality is of lower order and can hence be absorbed into the second term in form of a multiplicative constant μ_n slightly larger than one, so that we need $\frac{2\mu_n}{n}(v^\top \tilde{\beta})^2 < (1 - \delta)^2/4$, or equivalently,

$$v^\top \tilde{\beta} \leq \frac{1 - \delta}{\sqrt{8\mu_n}}\sqrt{n}$$

Conditional on E_1 to E_4 , inserting the bound on $\mathbf{1}^\top \tilde{\beta}$ in (B.3) shows that we need

$$r_{\nu,p} \geq \sqrt{8\mu_n} \frac{1 + \delta}{1 - \delta} C_2^{-1} \left(\sqrt{\frac{2}{\pi}} + C_3 \right),$$

which can be achieved by taking $p/n \geq C_0$ for a sufficiently large constant C_0 . Combining this with the probability estimates for the events E_1, \dots, E_4 , the proof is complete.

APPENDIX C: PROOF OF THEOREM 3

Since $\hat{\beta}$ is a minimizer of the NNLS problem (1.2) and since β^* is a feasible solution, we have that

$$\begin{aligned} \frac{1}{n}\|y - X\hat{\beta}\|_2^2 &\leq \frac{1}{n}\|y - X\beta^*\|_2^2 \\ \Leftrightarrow \|(f + \varepsilon - X\beta^*) + X\beta^* - X\hat{\beta}\|_2^2 &\leq \frac{1}{n}\|f + \varepsilon - X\beta^*\|_2^2 \\ \Rightarrow \frac{1}{n}\|X\beta^* - X\hat{\beta}\|_2^2 + \frac{2}{n}(f + \varepsilon - X\beta^*)^\top X(\beta^* - \hat{\beta}) &\leq 0 \\ \Rightarrow \frac{1}{n}\|X\beta^* - X\hat{\beta}\|_2^2 &\leq \frac{2}{n}(f - X\beta^*)^\top X(\hat{\beta} - \beta^*) + \frac{2}{n}\varepsilon^\top X(\hat{\beta} - \beta^*). \end{aligned} \tag{C.1}$$

Write $\widehat{\delta} = \widehat{\beta} - \beta^*$, $P = \{j : \widehat{\delta}_j \geq 0\}$ and $N = \{j : \widehat{\delta}_j < 0\}$. We now lower bound $\frac{1}{n}\|X\widehat{\delta}\|_2^2 = \widehat{\delta}^\top \Sigma \widehat{\delta}$ using the self-regularizing property (2.5).

$$(C.2) \quad \begin{aligned} \frac{1}{n}\|X\widehat{\delta}\|_2^2 &= \widehat{\delta}_P^\top \Sigma_{PP} \widehat{\delta}_P + 2\widehat{\delta}_P^\top \Sigma_{PN} \widehat{\delta}_N + \widehat{\delta}_N^\top \Sigma_{NN} \widehat{\delta}_N \\ &\geq \tau_0^2 (\mathbf{1}^\top \widehat{\delta}_P)^2 - 2\|\widehat{\delta}_P\|_1 \|\widehat{\delta}_N\|_1. \end{aligned}$$

Second, we bound the r.h.s. of (C.1). We set $A = \max_{1 \leq j \leq p} \left| \frac{1}{n} X_j^\top \varepsilon \right|$ and use the bound

$$\max_{1 \leq j \leq p} \left| \frac{1}{n} X_j^\top (f - X\beta^*) \right| \leq \max_{1 \leq j \leq p} \frac{1}{\sqrt{n}} \|X_j\|_2 \sqrt{\frac{1}{n} \|f - X\beta^*\|_2^2} = \sqrt{\mathcal{E}^*},$$

obtaining that

$$(C.3) \quad \frac{1}{n}\|X\widehat{\delta}\|_2^2 \leq 2(A + \sqrt{\mathcal{E}^*})\|\widehat{\delta}\|_1$$

Inserting the lower bound (C.2) into (C.3), we obtain

$$(C.4) \quad \tau_0^2 \|\widehat{\delta}_P\|_1^2 - 2\|\widehat{\delta}_P\|_1 \|\widehat{\delta}_N\|_1 \leq 2(A + \sqrt{\mathcal{E}^*})(\|\widehat{\delta}_P\|_1 + \|\widehat{\delta}_N\|_1).$$

We may assume that $\widehat{\delta}_P \neq 0$, otherwise the assertion of the theorem would follow immediately, because $\|\widehat{\delta}_N\|_1$ is already bounded for feasibility reasons, see below. Dividing both sides by $\|\widehat{\delta}_P\|_1$ and re-arranging yields

$$(C.5) \quad \|\widehat{\delta}_P\|_1 \leq \frac{4(A + \sqrt{\mathcal{E}^*}) + 2\|\widehat{\delta}_N\|_1}{\tau_0^2},$$

where we have assumed that $\|\widehat{\delta}_N\|_1 \leq \|\widehat{\delta}_P\|_1$ (if that were not the case, one would obtain $\|\widehat{\delta}_P\|_1 \leq \|\widehat{\delta}_N\|_1$, which is stronger than (C.5), since $0 < \tau_0^2 \leq 1$). We now substitute (C.5) back into (C.1) and add $\mathcal{E}^* = \frac{1}{n}\|X\beta^* - f\|_2^2$ to both sides of the inequality in order to obtain

$$\begin{aligned} \widehat{\mathcal{E}} = \frac{1}{n}\|X\widehat{\beta} - f\|_2^2 &\leq \mathcal{E}^* + 2A(\|\widehat{\delta}_P\|_1 + \|\widehat{\delta}_N\|_1) \\ &\leq \mathcal{E}^* + 2A \left(\frac{4(A + \sqrt{\mathcal{E}^*}) + 2\|\widehat{\delta}_N\|_1}{\tau_0^2} + \|\widehat{\delta}_N\|_1 \right) \\ &\leq \mathcal{E}^* + \frac{6A\|\beta^*\|_1 + 8(A^2 + A\sqrt{\mathcal{E}^*})}{\tau_0^2}, \end{aligned}$$

noting that by feasibility of $\widehat{\beta}$, one has $\widehat{\delta} \succeq -\beta^*$ and hence $\|\widehat{\delta}_N\|_1 \leq \|\beta^*\|_1$. Using the maximal inequality (A.2) for a finite collection of sub-Gaussian random variables, the event $\left\{ A \leq 2\sigma \sqrt{\frac{2\log p}{n}} \right\}$ holds with probability no less than $1 - 2/p$. The result follows.

APPENDIX D: PROOF OF THEOREM 4

Arguing similarly as in the proof of Theorem 3, it will be shown that $\|\widehat{\delta}_{S^c}\|_1 \leq \frac{3}{\tau_0} \|\widehat{\delta}_S\|_1$, i.e. $\widehat{\delta} \in \mathcal{R}(3/\tau_0^2, S)$ as defined in Condition 2; in the sequel,

all notation introduced in the previous proof are adopted. Note that $S^c \subseteq P$ and $N \subseteq S$. Hence, we obtain the following analog to (C.4).

$$\tau_0^2 \|\widehat{\delta}_{S^c}\|_1^2 - 2\|\widehat{\delta}_{S^c}\|_1 \|\widehat{\delta}_S\|_1 \leq 2A(\|\widehat{\delta}_S\|_1 + \|\widehat{\delta}_{S^c}\|_1).$$

Dividing both sides by $\|\widehat{\delta}_{S^c}\|_1$, assuming that $0 < \|\widehat{\delta}_S\|_1 \leq \|\widehat{\delta}_{S^c}\|_1$ (otherwise, the claim $\widehat{\delta} \in \mathcal{R}(3/\tau_0^2, S)$ would follow trivially), we obtain

$$\tau_0^2 \|\widehat{\delta}_{S^c}\|_1 \leq 4A + 2\|\widehat{\delta}_S\|_1 \leq 3\|\widehat{\delta}_S\|_1,$$

assuming that $4A \leq \|\widehat{\delta}_S\|_1$, i.e. $\widehat{\delta} \in \mathcal{R}(3/\tau_0^2, S)$. Suppose conversely that $\|\widehat{\delta}_S\|_1 \leq 4A$. One then has

$$\|\widehat{\delta}_{S^c}\|_1 \leq \frac{12A}{\tau_0^2}, \quad \frac{1}{n} \|X\widehat{\delta}\|_2^2 \leq 2A \left\{ \frac{12A}{\tau_0^2} + 4A \right\},$$

so that the assertion of Theorem 4 follows. Conditional on $\widehat{\delta} \in \mathcal{R}(3/\tau_0^2, S)$, one may invoke the compatibility condition (2.10), which, when applied to (C.1), yields

$$s^{-1} \phi \left(\frac{3}{\tau_0^2}, S \right) \|\widehat{\delta}_S\|_1^2 \leq \frac{1}{n} \|X\widehat{\delta}\|_2^2 \leq 2A(\|\widehat{\delta}_S\|_1 + \|\widehat{\delta}_{S^c}\|_1) \leq \frac{8A}{\tau_0^2} \|\widehat{\delta}_S\|_1$$

which implies that

$$\begin{aligned} \|\widehat{\delta}_S\|_1 &\leq \frac{8A s}{\tau_0^2 \phi \left(\frac{3}{\tau_0^2}, S \right)}, \quad \|\widehat{\beta} - \beta^*\|_1 = \|\widehat{\delta}\|_1 \leq \frac{32A s}{\tau_0^4 \phi \left(\frac{3}{\tau_0^2}, S \right)}, \\ \frac{1}{n} \|X\widehat{\beta} - X\beta^*\|_2^2 &\leq \frac{64A^2 s}{\tau_0^4 \phi \left(\frac{3}{\tau_0^2}, S \right)}. \end{aligned}$$

We conclude by applying (A.2) as in Theorem 1.

APPENDIX E: PROOF OF THEOREM 6

E.1. $\tau^2(S)$ for equi-correlation. We first prove (3.12) for the population Gram matrix $\Sigma^* = \mathbf{E}[\frac{1}{n} X^\top X] = \rho I + (1 - \rho) \mathbf{1}\mathbf{1}^\top$, $\rho \in (0, 1)$. We compute $\tau^2(S) = \tau^2(s)$ from the matrix $\frac{1}{n} Z^\top Z$ via (3.3). One computes that

$$(E.1) \quad (\Sigma_{SS}^{-1})_{jk} = \frac{1}{(1 - \rho)(1 + (s - 1)\rho)} \begin{cases} 1 + (s - 2)\rho & j = k, \\ -\rho & j \neq k. \end{cases}$$

and consequently, using (3.22),

$$(E.2) \quad \left(\frac{1}{n} Z^\top Z \right)_{jk} = \begin{cases} 1 - \rho^2 s / (1 + (s - 1)\rho) & j = k, \\ \rho - \rho^2 s / (1 + (s - 1)\rho) & j \neq k. \end{cases}$$

In view of the simple structure (E.2), one verifies that the minimum in (3.3) is attained for $\lambda = 1/(p - s)$, which yields that

$$\tau^2(s) = \frac{(1 - \rho)\rho}{(s - 1)\rho + 1} + \frac{1 - \rho}{p - s},$$

as was to be shown.

We state and prove three lemmas first, which rely on the following two theorems that can be found in [46].

E.2. Bernstein-type inequality for squared sub-Gaussian random variables. The following exponential inequality combines Lemma 14, Proposition 16 and Remark 18 in [46].

THEOREM D. 1. *Let Z_1, \dots, Z_n be i.i.d. centered sub-Gaussian random variables with sub-Gaussian norm K . Then for every $a = (a_1, \dots, a_n)^\top \in \mathbb{R}^n$ and every $z \geq 0$, one has*

$$(E.3) \quad \mathbf{P} \left(\left| \sum_{i=1}^n a_i (Z_i^2 - \mathbf{E}[Z_i^2]) \right| > z \right) \leq 2 \exp \left(-c \min \left(\frac{z^2}{K^4 \|a\|_2^2}, \frac{z}{K^2 \|a\|_\infty} \right) \right),$$

where $c > 0$ is an absolute constant.

E.3. Concentration of extreme singular values of sub-Gaussian random matrices. Recall that $s_{\min}(X)$ and $s_{\max}(X)$ denote the minimum and maximum singular value of a matrix X . The following statement, which is a generalization of Theorem 2, is a special case covered by Theorem 39 in [46].

THEOREM D. 2. *Let X be an $n \times s$ matrix with i.i.d. centered sub-Gaussian entries having unit variance and sub-Gaussian norm K . Then for every $z \geq 0$, with probability at least $1 - 2 \exp(-cz^2)$, one has*

$$(E.4) \quad \sqrt{n} - C\sqrt{s} - z \leq s_{\min}(X) \leq s_{\max}(X) \leq \sqrt{n} + C\sqrt{s} + z, \text{ and}$$

$$(E.5) \quad s_{\max} \left(\frac{1}{n} X^\top X - I \right) \leq \max(\delta, \delta^2), \text{ where } \delta = C \sqrt{\frac{s}{n}} + \frac{z}{\sqrt{n}},$$

with C, c depending only on K .

E.4. Additional lemmas.

LEMMA D. 1. *Let Z_1, \dots, Z_n be i.i.d. centered, unit variance sub-Gaussian random variables with sub-Gaussian norm K . Then for all $z \geq 0$*

$$(E.6) \quad \mathbf{P} \left(\sum_{i=1}^n Z_i^2 > n + zn \right) \leq \exp(-c \min(\frac{z^2}{K^4}, \frac{z}{K^2})n).$$

PROOF. Noting that $\mathbf{E}[\sum_{i=1}^n Z_i^2] = n$ and re-arranging, the result follows from Theorem D.1 with $a = (1, \dots, 1)^\top$. \square

In the sequel, we denote by Σ^* the population covariance $\mathbf{E}[\frac{1}{n} X^\top X] = (1 - \rho)I_p + \rho \mathbf{1}\mathbf{1}^\top$, where $\rho \in (0, 1)$ depends on the specific distribution for the entries (x_{ij}) .

LEMMA D. 2. *If X is a random matrix from Ens_+ (3.13), then for all $t \geq 0$ and any $S \subseteq \{1, \dots, p\}$, $|S| \leq s$, with probability at least $1 - 2 \exp(-c_1 t^2) - \exp(-c_2 \min(t^2, t)s)$*

$$(E.7) \quad s_{\max} \left(\frac{1}{n} X_S^\top X_S - \Sigma_{SS}^* \right) \leq \max(\delta, \delta^2) + C_1 \sqrt{\frac{s^2(1+t)}{n}}, \quad \delta = C_2 \sqrt{\frac{s}{n}} + \frac{t}{\sqrt{n}},$$

where $C, C_1, C_2, c, c_1, c_2 > 0$ are universal constants.

PROOF. We decompose the rows $\{X_S^i\}_{i=1}^n$ of X_S as $X_S^i = \tilde{X}_S^i + \mu \mathbf{1}$, where $\mu > 0$ is the mean of the entries, $i = 1, \dots, n$. We have

$$\begin{aligned} s_{\max} \left(\frac{1}{n} X_S^\top X_S - \Sigma_{SS}^* \right) &= \sup_{\|v\|_2=1} \left| \frac{1}{n} \sum_{i=1}^n \left(\langle \tilde{X}_S^i + \mu \mathbf{1}, v \rangle^2 - \mathbf{E}[\langle \tilde{X}_S^i + \mu \mathbf{1}, v \rangle^2] \right) \right|, \\ &= \sup_{\|v\|_2=1} \left| \frac{1}{n} \sum_{i=1}^n \left(\langle \tilde{X}_S^i, v \rangle^2 - \mathbf{E}[\langle \tilde{X}_S^i, v \rangle^2] + 2 \langle \mu \mathbf{1}, v \rangle \langle \tilde{X}_S^i, v \rangle \right) \right| \\ &\leq \sup_{\|v\|_2=1} \left| \frac{1}{n} \sum_{i=1}^n \left(\langle \tilde{X}_S^i, v \rangle^2 - \mathbf{E}[\langle \tilde{X}_S^i, v \rangle^2] \right) \right| + 2 \sup_{\|v\|_2=1} \left| \langle \mu \mathbf{1}, v \rangle \frac{1}{n} \sum_{i=1}^n \langle \tilde{X}_S^i, v \rangle \right| \end{aligned}$$

The first summand is handled by an application of Theorem D.2. For the second summand, we have

$$2 \sup_{v: \|v\|_2=1} \left| \langle \mu \mathbf{1}, v \rangle \frac{1}{n} \sum_{i=1}^n \langle \tilde{X}_S^i, v \rangle \right| \leq 2 \left| \mu \sqrt{s} \left\| \frac{1}{n} \sum_{i=1}^n \tilde{X}_S^i \right\|_2 \right|.$$

Re-writing the norm as

$$\left\| \frac{1}{n} \sum_{i=1}^n \tilde{X}_S^i \right\|_2 = \left(\frac{1}{n} \sum_{j \in S} \left(\frac{1}{\sqrt{n}} \sum_{i=1}^n \tilde{x}_{ij} \right)^2 \right)^{1/2} = \left(\frac{1}{n} \sum_{j=1}^s Z_j^2 \right)^{1/2}, \quad Z_j = \frac{1}{\sqrt{n}} \sum_{i=1}^n \tilde{x}_{ij}.$$

and noting that, as explained in Appendix A, the sub-Gaussian norm of the $\{Z_j\}$ is uniformly bounded by an absolute constant, say L , we invoke (E.6), which yields for all $t \geq 0$

$$\mathbf{P} \left(\sum_{j=1}^s Z_j^2 > s + ts \right) \leq \exp \left(-c \min \left(\frac{t^2}{L^4}, \frac{t}{L^2} \right) s \right).$$

The claim follows by taking roots and back-substituting. \square

LEMMA D. 3.

$$\max_{1 \leq j, k \leq p} \left| \left(\frac{1}{n} X^\top X - \Sigma^* \right)_{jk} \right| \leq C \sqrt{\frac{\log p}{n}},$$

with probability at least $1 - 3/p - \exp(-cn)$, where $C, c > 0$ are universal constants.

PROOF. Write $\tilde{X}_j = X_j - \mu \mathbf{1}$, $j = 1, \dots, p$, for the column vectors obtained by centering the columns of X . We have

$$(E.8) \quad \frac{1}{n} (\langle X_j, X_k \rangle - \mathbf{E}[\langle X_j, X_k \rangle]) = \frac{1}{n} \langle \tilde{X}_j, \tilde{X}_k \rangle - \mu \left(\frac{1}{n} \langle \tilde{X}_j, \mathbf{1} \rangle + \frac{1}{n} \langle \tilde{X}_k, \mathbf{1} \rangle \right).$$

For the second term in (E.8), we have, in view of the properties of sub-Gaussian random variables in Appendix A

$$(E.9) \quad \mathbf{P} \left(\left| \frac{\mu}{n} \langle \tilde{X}_j + \tilde{X}_k, \mathbf{1} \rangle \right| > \sqrt{2} \mu z \right) \leq 2 \exp(-c_0 n z^2).$$

For the first term in (E.8), let us first consider the case $j \neq k$. Fix any $j \in \{1, \dots, p\}$. It follows from Lemma F.1 that the event $\mathcal{E}_j = \{\|X_j\|_2^2 \leq 2n\}$ holds

with probability at least $1 - \exp(-c_1 n)$. Conditional on \mathcal{E}_j , $\langle \tilde{X}_j, \tilde{X}_k \rangle$ is a sub-Gaussian random variable with sub-Gaussian norm bounded by $L\sqrt{n}$, for some universal constant $L > 0$. It follows that

$$(E.10) \quad \begin{aligned} \mathbf{P} \left(\left| \frac{1}{n} \langle \tilde{X}_j, \tilde{X}_k \rangle \right| > z \right) &\leq \mathbf{P} \left(\left| \frac{1}{n} \langle \tilde{X}_j, \tilde{X}_k \rangle \right| > z \middle| \mathcal{E}_j \right) + \mathbf{P}(\mathcal{E}_j^c) \\ &\leq 2 \exp(-c_2 n z^2 / L^2) + \exp(-c_1 n) \leq 2 \exp(-c_3 n z^2) + \exp(-c_1 n). \end{aligned}$$

Let now $j = k$. With the aim to control the first term in (E.8), an application of Theorem D.1 yields $\forall z \geq 0$

$$(E.11) \quad \mathbf{P} \left(\left| \frac{1}{n} \sum_{j=1}^n (\tilde{x}_{ij}^2 - \mathbf{E}[\tilde{x}_{ij}^2]) \right| > z \right) \leq 2 \exp(-c_4 \min(z, z^2)n).$$

Combining (E.9), (E.10) and (E.11), with a union bound over all p^2 entries of $\frac{1}{n} X^\top X$ and setting $z = 2/\sqrt{\min\{c_0, c_3, c_4\}} \sqrt{\frac{\log p}{n}}$, we obtain

$$\mathbf{P} \left(\left| \left(\frac{1}{n} X^\top X - \Sigma^* \right)_{jk} \right| > C \sqrt{\frac{\log p}{n}} \right) \leq \frac{3}{p} + \exp(-c_1 n + \log p).$$

□

Proof of Theorem 6. Equipped with these auxiliary results, we turn to the actual proof of the Theorem. We analyze the random scaling of $\tau^2(S)$ using the dual formulation (3.3). In the following, denote by $\mathbb{S}^{s-1} = \{u \in \mathbb{R}^s : \|u\|_2 = 1\}$ the unit sphere in \mathbb{R}^s . Expanding the square in (3.3), we have

$$(E.12) \quad \begin{aligned} \tau^2(S) &= \min_{\theta \in \mathbb{R}^s, \lambda \in T^{p-s-1}} \theta^\top \frac{1}{n} X_S^\top X_S \theta - 2\theta^\top \frac{1}{n} X_S^\top X_{S^c} \lambda + \lambda^\top \frac{1}{n} X_{S^c}^\top X_{S^c} \lambda \\ &\geq \min_{r>0, u \in \mathbb{S}^{s-1}, \lambda \in T^{p-s-1}} r^2 u^\top \Sigma_{SS}^* u - r^2 s_{\max} \left(\frac{1}{n} X_S^\top X_S - \Sigma_{SS}^* \right) - \\ &\quad - 2ru^\top \frac{1}{n} X_S^\top X_{S^c} \lambda + \lambda^\top \frac{1}{n} X_{S^c}^\top X_{S^c} \lambda \\ &\geq \min_{r>0, u \in \mathbb{S}^{s-1}, \lambda \in T^{p-s-1}} r^2 u^\top \Sigma_{SS}^* u - r^2 s_{\max} \left(\frac{1}{n} X_S^\top X_S - \Sigma_{SS}^* \right) \\ &\quad - 2\rho r u^\top \mathbf{1} - 2ru^\top \left(\frac{1}{n} X_S^\top X_{S^c} - \Sigma_{SS^c}^* \right) \lambda + \rho + \frac{1-\rho}{p-s} \\ &\quad - \sup_{\lambda \in T^{p-s-1}} \left| \lambda^\top \left(\frac{1}{n} X_{S^c}^\top X_{S^c} - \Sigma_{S^c S^c}^* \right) \lambda \right|. \end{aligned}$$

For the last inequality, we have used that $\min_{\lambda \in T^{p-s-1}} \lambda^\top \Sigma_{S^c S^c}^* \lambda = \rho + \frac{1-\rho}{p-s}$ by setting $\lambda = \mathbf{1}/(p-s)$. We further set $\Delta = s_{\max} \left(\frac{1}{n} X_S^\top X_S - \Sigma_{SS}^* \right)$ and $\delta = \sup_{u \in \mathbb{S}^{s-1}, \lambda \in T^{p-s-1}} \left| u^\top \left(\frac{1}{n} X_{S^c}^\top X_{S^c} - \Sigma_{S^c S^c}^* \right) \lambda \right|$. The random deviation terms Δ and δ will be controlled uniformly over $u \in \mathbb{S}^{s-1}$ and $\lambda \in T^{p-s-1}$ by means of the two preceding lemmas, and are hence subsequently treated as constants. This approach allows us to minimize the lower bound in (E.12) w.r.t. u and r separately from λ . The minimization problem involving u and r reads

$$(E.13) \quad \min_{r>0, u \in \mathbb{S}^{s-1}} r^2 u^\top \Sigma_{SS}^* u - 2\rho r u^\top \mathbf{1} - r^2 \Delta - 2r\delta.$$

We first derive an expression for

$$(E.14) \quad \phi(r) = \min_{u \in \mathbb{S}^{s-1}} r^2 u^\top \Sigma_{SS}^* u - 2\rho r u^\top \mathbf{1}.$$

We decompose $u = u^\parallel + u^\perp$, where $u^\parallel = \left\langle \frac{\mathbf{1}}{\sqrt{s}}, u \right\rangle \frac{\mathbf{1}}{\sqrt{s}}$ is the projection of u on the unit vector $\mathbf{1}/\sqrt{s}$, which is the eigenvector of Σ_{SS}^* associated with its largest eigenvalue $1 + \rho(s-1)$. By Parseval's identity, we have $\|u^\parallel\|_2^2 = \gamma$, $\|u^\perp\|_2^2 = (1 - \gamma)$ for some $\gamma \in [0, 1]$. Inserting this decomposition and noting that the remaining eigenvalues of Σ_{SS}^* are all equal to $(1 - \rho)$, we obtain the following expression to be minimized w.r.t. $\gamma \in [0, 1]$

$$(E.15) \quad r^2 \underbrace{\gamma(1 + (s-1)\rho)}_{s_{\max}(\Sigma_{SS}^*)} + r^2(1 - \gamma) \underbrace{(1 - \rho)}_{s_{\min}(\Sigma_{SS}^*)} - 2\rho r \sqrt{\gamma} \sqrt{s},$$

where we have used that $\langle u^\perp, \mathbf{1} \rangle = 0$ and that all potential minimizers must satisfy $\langle u^\parallel, \mathbf{1} \rangle > 0$. Let us put aside the constraint $\gamma \in [0, 1]$ for a moment. The expression (E.15) is a convex function of γ , hence we may find an (unconstrained) minimizer $\tilde{\gamma}$ by differentiating and setting the derivative equal to zero. This yields $\tilde{\gamma} = \frac{1}{r^2 s}$, which coincides with the constrained minimizer if and only if $r \geq \frac{1}{\sqrt{s}}$. Now observe that the minimizer of the problem $\min_{r>0, u \in \mathbb{S}^{s-1}} r^2 u^\top \Sigma_{SS}^* u - 2\rho r u^\top \mathbf{1}$ with r being unfixed equals the minimizer $\hat{\theta}$ of the problem $\min_{\theta \in \mathbb{R}^s} \theta^\top \Sigma_{SS}^* \theta - 2\rho \theta^\top \mathbf{1}$, which is given by $\hat{\theta} = \frac{\rho \mathbf{1}}{1 + (s-1)\rho} = \frac{1}{\sqrt{s}} \cdot \frac{\sqrt{s}\rho}{1 + (s-1)\rho}$, a unit vector satisfying $\gamma = 1$ times a radius less than $1/\sqrt{s}$. We conclude that for all $r < 1/\sqrt{s}$, the minimum is attained for $\gamma = 1$, hence the function $\phi(r)$ (E.14) is given by

$$(E.16) \quad \phi(r) = \begin{cases} r^2 s_{\max}(\Sigma_{SS}^*) - 2\rho r \sqrt{s} & r < 1/\sqrt{s}, \\ r^2(1 - \rho) - \rho & \text{otherwise,} \end{cases}$$

where the second line is obtained by inserting $\tilde{\gamma} = \frac{1}{r^2 s}$ for γ in (E.15). The minimization problem (E.13) to be considered eventually reads

$$(E.17) \quad \min_{r>0} \psi(r), \quad \psi(r) = \phi(r) - r^2 \Delta - 2r\delta.$$

We argue that it suffices to consider the case $r < 1/\sqrt{s}$ in (E.16) provided

$$(E.18) \quad ((1 - \rho) - \Delta)^2 > \delta^2 s,$$

a condition we will comment on below. If this condition is met, differentiating shows that ψ is increasing on $[\frac{1}{\sqrt{s}}, \infty)$. In fact, for all r in that ray,

$$\frac{d}{dr} \psi(r) = 2r(1 - \rho) - 2r\Delta - 2\delta, \text{ and thus}$$

$$\frac{d}{dr} \psi(r) > 0 \text{ for all } r \in \left[\frac{1}{\sqrt{s}}, \infty \right) \Leftrightarrow \frac{1}{\sqrt{s}}((1 - \rho) - \Delta) > \delta \Leftrightarrow ((1 - \rho) - \Delta)^2 > s\delta^2.$$

Considering the case $r < 1/\sqrt{s}$, we observe that $\psi(r)$ is convex provided

$$(E.19) \quad s_{\max}(\Sigma_{SS}^*) > \Delta,$$

a condition we shall comment on below as well. Provided (E.18) and (E.19) hold true, the minimizer \hat{r} of (E.17) is given by $(\rho\sqrt{s} + \delta)/(s_{\max}(\Sigma_{SS}^*) - \Delta)$. Substituting this result back into (E.17) and in turn into the lower bound (E.12), one obtains after collecting terms

$$(E.20) \quad \tau^2(S) \geq \rho \frac{(1-\rho) - \Delta}{(1-\rho) + s\rho - \Delta} - \frac{2\rho\sqrt{s}\delta + \delta^2}{s_{\max}(\Sigma_{SS}^*) - \Delta} + \frac{1-\rho}{p-s} - \sup_{\lambda \in T^{p-s-1}} \left| \lambda^\top \left(\frac{1}{n} X_{S^c}^\top X_{S^c} - \Sigma_{S^c S^c}^* \right) \lambda \right|.$$

Consider the two events

$$\mathcal{A} = \left\{ \Delta \leq C_1 \left(\sqrt{\frac{s^2 \log^{1/2} p}{n}} + \sqrt{\frac{\log p}{n}} \right) \right\}, \mathcal{B} = \left\{ \max_{j,k} \left| \left(\frac{1}{n} X^\top X - \Sigma^* \right)_{jk} \right| \leq C_2 \sqrt{\frac{\log p}{n}} \right\},$$

for universal constants $C_1, C_2 > 0$. Conditional on $\mathcal{A} \cap \mathcal{B}$, bounding

$$\delta \leq \sup_{u \in \mathbb{S}^{s-1}} \|u\|_1 \sup_{\lambda \in T^{p-s-1}} \left\| \left(\frac{1}{n} X_{S^c}^\top X_{S^c} - \Sigma_{S^c S^c}^* \right) \lambda \right\|_\infty \leq \sqrt{s} C_2 \sqrt{\frac{\log p}{n}},$$

and inserting the scaling for Δ under \mathcal{A} , there exists a sufficiently large constant $\hat{C} > 0$ such that the two conditions (E.18) and (E.19) supposed to be fulfilled previously indeed hold given that $n \geq \hat{C} \log(p) s^2$. We may re-write (E.20) as

$$(E.21) \quad \tau^2(S) \geq \frac{\rho(1 - \Delta/(1-\rho))}{(1 - \Delta/(1-\rho)) + s \frac{\rho}{1-\rho}} + \frac{2\rho \frac{\sqrt{s}}{1+(s-1)\rho} \delta}{1 - \Delta/(1+(s-1)\rho)} - \frac{\delta^2/(1+(s-1)\rho)}{1 - \Delta/(1+(s-1)\rho)} - \sup_{\lambda \in T^{p-s-1}} \left| \lambda^\top \left(\frac{1}{n} X_{S^c}^\top X_{S^c} - \Sigma_{S^c S^c}^* \right) \lambda \right|.$$

Conditional on $\mathcal{A} \cap \mathcal{B}$, there exists again a sufficiently large constant $\tilde{C} > 0$ such that if $n \geq \tilde{C} \log(p) s^2$

$$(E.22) \quad c_1 \frac{1}{s} - C_3 \sqrt{\frac{\log p}{n}} - C_4 \frac{\log p}{n} - C_2 \sqrt{\frac{\log p}{n}} = c_1 \frac{1}{s} - C_5 \sqrt{\frac{\log p}{n}}$$

by inserting the resulting scalings separately for each summand in (E.21), where $c_1, C_3, C_4, C_5 > 0$ are universal constants. We conclude that if $n \geq \max(\hat{C}, \tilde{C}) \log(p) s^2$, (E.22) holds with probability no less than $1 - \mathbf{P}(\mathcal{A}) - \mathbf{P}(\mathcal{B})$. Using Lemmas F.2 and F.3 to control $\mathbf{P}(\mathcal{A})$ and $\mathbf{P}(\mathcal{B})$, the result follows.

APPENDIX F: PROPERTIES OF THE CONSTANT $\omega(S)$

In this section, we derive the following three properties.

- (i) $\omega(S) > 0 \Leftrightarrow \tau(S) > 0 \Leftrightarrow X_S \mathbb{R}_+^s$ is a face of \mathcal{C} ,
- (ii) $\omega(S) \leq 1$, with equality if $\{X_j\}_{j \in S} \perp \{X_j\}_{j \in S^c}$ and $\frac{1}{n} X_{S^c}^\top X_{S^c} \succeq 0$
- (iii) $\omega(S) \geq \min_{1 \leq j \leq (p-s)} \frac{1}{n} (Z^\top Z)_{jj} + \frac{1}{n} \sum_{k \neq j} \min\{(Z^\top Z)_{jk}, 0\},$

PROOF. (i): From (3.3), we have

$$(F.1) \quad \tau^2(S) = \min_{\lambda \in T^{p-s-1}} \frac{1}{n} \|Z\lambda\|_2^2, \text{ hence}$$

$$\exists \hat{\lambda} \in T^{p-s-1} \text{ s.t. } Z\hat{\lambda} = 0 \Rightarrow Z^\top Z\hat{\lambda} = 0 \Rightarrow \|Z^\top Z\hat{\lambda}\|_\infty = 0 \Rightarrow \omega(S) = 0.$$

On the other hand

$$\exists \hat{v} \in \mathcal{V}(F) \text{ s.t. } \|Z_F^\top Z_F \hat{v}\|_\infty = 0 \Rightarrow Z_F^\top Z_F \hat{v} = 0 \Rightarrow \|Z_F \hat{v}\|_2^2 \Rightarrow \tau(S) = 0.$$

The second equivalence is by the definition of a face of a cone.

(ii) Consider all principal sub-matrices $\frac{1}{n}Z_F^\top Z_F$. By definition, $\omega(S)$ equals the maximum of the absolute values of the entries of $\frac{1}{n}Z_F^\top Z_F v$, where one minimizes over all v contained in the boundary of the unit cube $[0, 1]^{|F|}$. We may restrict our attention to matrices $\frac{1}{n}Z^\top Z$ which are entry-wise non-negative. To see this, assume that there exists a non-negative off-diagonal entry for a pair (j, k) . Then pick $F_0 = \{j, k\}$ and set $\mathcal{V}(F_0) = \{v \in \mathbb{R}^2 : v \succeq 0, \|v\|_\infty = 1\}$ to obtain that

$$\begin{aligned} \omega(S) &\leq \min_{v \in \mathcal{V}(F_0)} \left\| \frac{1}{n} Z_{F_0}^\top Z_{F_0} v \right\|_\infty \leq \max \left\{ \frac{1}{n} (Z^\top Z)_{jj} + \frac{1}{n} (Z^\top Z)_{jk}, \right. \\ &\quad \left. \frac{1}{n} (Z^\top Z)_{kk} + \frac{1}{n} (Z^\top Z)_{jk} \right\} \\ &\leq \max \left\{ \frac{1}{n} (Z^\top Z)_{jj}, \frac{1}{n} (Z^\top Z)_{kk} \right\} \leq 1, \end{aligned}$$

re-calling that $\|Z_j\|_2^2 = \|\Pi_S^\perp X_j\|_2^2 \leq \|X_j\|_2^2 = n$ for all j . If $Z^\top Z$ is entry-wise non-negative, a similar argument shows that $\omega(S)$ equals the minimum diagonal entry of $\frac{1}{n}Z^\top Z$, which is upper bounded by 1. Using expansion (3.22), we may write

$$\frac{1}{n}Z^\top Z = \frac{1}{n}X_{S^c}^\top X_{S^c} - \frac{1}{n}X_{S^c}^\top X_S \left(\frac{1}{n}X_S^\top X_S \right)^{-1} X_S^\top X_{S^c},$$

orthogonality implies that $\frac{1}{n}Z^\top Z = \frac{1}{n}X_{S^c}^\top X_{S^c}$. Using entry-wise non-negativity of $\frac{1}{n}X_{S^c}^\top X_{S^c}$ together with $\|X_j\|_2^2 = n$ for all j , the assertion follows.

(iii) can be derived directly from the definition of $\omega(S)$:

$$\begin{aligned} \omega(S) &= \min_{\emptyset \neq F \subseteq \{1, \dots, p-s\}} \min_{v \in \mathcal{V}(F)} \left\| \frac{1}{n} Z_F^\top Z_F v \right\|_\infty, \quad \mathcal{V}(F) = \{v \in \mathbb{R}^{|F|} : \|v\|_\infty = 1, v \succeq 0\}. \\ &= \min_{\emptyset \neq F \subseteq \{1, \dots, p-s\}} \min_{v \in \mathcal{V}(F)} \max_{j \in F} \frac{1}{n} \left| (Z^\top Z)_{jj} v_j + \sum_{k \neq j} (Z^\top Z)_{jk} v_k \right| \\ &\geq \min_{\emptyset \neq F \subseteq \{1, \dots, p-s\}} \min_{j \in F} \min_{\{v_k : 0 \leq v_k \leq 1\}} \frac{1}{n} \left((Z^\top Z)_{jj} + \sum_{k \neq j} (Z^\top Z)_{jk} v_k \right) \\ &= \min_{\emptyset \neq F \subseteq \{1, \dots, p-s\}} \min_{j \in F} \frac{1}{n} \left((Z^\top Z)_{jj} + \sum_{k \neq j} \min\{(Z^\top Z)_{jk}, 0\} \right) \\ &= \min_{1 \leq j \leq (p-s)} \frac{1}{n} \left((Z^\top Z)_{jj} + \sum_{k \neq j} \min\{(Z^\top Z)_{jk}, 0\} \right) \end{aligned}$$

□

APPENDIX G: PROOF OF THEOREM 9

The proof is along the lines of [22] (proof of their Theorem 3). Note that in the setting of Theorem 7 or 8, if the condition imposed on $\beta_{\min}(S)$ in 9 holds true, the event $E = \{r_j \leq s, j \in S\}$ holds with probability tending to one. The probabilities of the two events

$$E_{>} = \{\widehat{s} > s\}, \quad E_{<} = \{\widehat{s} < s\}$$

are controlled separately. We have that

$$E_{>} \subseteq \bigcup_{k=s}^{p-1} \{\delta(k) > \widehat{\vartheta} \sqrt{2 \log n}\}$$

Conditional on E , each of the $\delta(k) = |u_k^\top \varepsilon|$, $k \geq s$, where u_k is a unit vector that spans the linear space $U_k = V_{k+1} \cap V_k^\perp$, where for $l = 1, \dots, p$, V_l is the linear spanned by the variables with rank no larger than l . Hence, the $\{\delta(k)\}$ follow sub-Gaussian distributions with expectation 1 and sub-Gaussian parameters depending only on the sub-Gaussian parameter σ of ε and a universal constant, so that $\mathbf{P}(\delta(k) > \widehat{\vartheta} \sqrt{2 \log n}) = o(1/n)$, by virtue of the assumption $\widehat{\vartheta} \geq c\vartheta$. Note that $\delta(k) = 0$ whenever $V_{k+1} = V_k$. Since X spans a subspace of dimension no larger than n , $\delta(k)$ can be nonzero no more than n times. By a union bound over the events $\{\delta(k) > \widehat{\vartheta} \sqrt{2 \log n}\}_{k=s}^{p-1}$, $\mathbf{P}(E_{>}|E) = o(1)$.

The probability of the event $E_{<}$ can be upper bounded by following the proof in [22] line by line, while noting that the slightly more general notion of sub-Gaussian noise ε can be accommodated easily.

APPENDIX H: PROOF OF THEOREM 10

Consider the non-negative lasso problem (3.29). It follows from the KKT optimality conditions that any minimizer $\widehat{\beta}^{\ell_{1,\succeq}}$ of (3.29) satisfies

(H.1)

$$2X_j^\top(y - X\widehat{\beta}^{\ell_{1,\succeq}}) = \lambda \text{ and } \widehat{\beta}_j^{\ell_{1,\succeq}} \geq 0, \quad 2X_j^\top(y - X\widehat{\beta}^{\ell_{1,\succeq}}) < \lambda \text{ and } \widehat{\beta}_j^{\ell_{1,\succeq}} = 0.$$

First note that λ_0 is chosen such that the event $\{\frac{1}{n}\|X^\top \varepsilon\|_\infty \leq \lambda_0\}$ holds with probability at least $1 - 2/p$. Subsequently, we work conditional on this event. Following the technique employed in [47], we establish that for $\lambda > 2\lambda_0/\gamma(S)$ with $\gamma(S)$ defined by (3.30), the unique minimizer is given by $\widehat{\beta}_S^{\ell_{1,\succeq}} = \widehat{\alpha}_S$ and $\widehat{\beta}_{S^c}^{\ell_{1,\succeq}} = 0$, where $\widehat{\alpha}$ denotes the minimizer of the following constrained non-negative lasso problem

$$\min_{\beta_S \succeq 0, \beta_{S^c} = 0} \frac{1}{n} \|y - X\beta\|_2^2 + \lambda \mathbf{1}^\top \beta.$$

To this end, in view of (H.1), we have to show that the following system of inequalities is satisfied

$$(H.2) \quad \frac{2}{n} \begin{bmatrix} X_S^\top \varepsilon \\ X_{S^c}^\top \varepsilon \end{bmatrix} + 2 \begin{bmatrix} \Sigma_{SS} & \Sigma_{SS^c} \\ \Sigma_{S^cS} & \Sigma_{S^cS^c} \end{bmatrix} \begin{bmatrix} \beta_S^* - \widehat{\alpha}_S \\ 0 \end{bmatrix} \begin{bmatrix} = \\ < \end{bmatrix} \begin{bmatrix} \lambda \mathbf{1} \\ \lambda \mathbf{1} \end{bmatrix}.$$

Using the lower bound on $\beta_{\min}(S)$ in (3.31), $\widehat{\alpha}_S \succ 0$ and we may resolve

$$\beta_S^* - \widehat{\alpha}_S = \frac{\lambda}{2} \Sigma_{SS}^{-1} \mathbf{1} - \Sigma_{SS}^{-1} \frac{1}{n} X_S^\top \varepsilon.$$

Substituting this into (H.2), we find that the following system of inequalities must hold true.

$$\frac{\lambda}{2} \{ \Sigma_{S^c S} \Sigma_{SS}^{-1} \mathbf{1} \} + \frac{1}{n} X_{S^c}^\top (I - \Pi_S) \varepsilon \prec \frac{\lambda}{2} \mathbf{1}.$$

Each component of the left hand side is no larger than $\frac{\lambda}{2}(1 - \gamma(S)) + \lambda_0$. It follows that for $\lambda > 2\lambda_0/\gamma(S)$, the system of inequalities is indeed fulfilled.

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